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Prediction of Properties of Silicon, Boron, and Aluminum Compounds

Kenneth H. Myers and Ronald P. Danner*

Department of Chemical Engineering, Pennsylvania State University, University Park, Pennsylvania 16802

Because of the lack of experimental results, organometallic compounds often have not been included in studies of data prediction methods. On the basis on an extensive search and compilation of experimental data, many of the thermodynamic and transport property prediction methods have now been extended to include silicon, boron, and aluminum compounds. Almost all the methods are based on chemical structure, involving atomic, bond, or group contributions. A strong emphasis has been placed on developing prediction methods of this type because a minimum number of experimental input data are required to apply them. This was an important criterion because of the scarcity of experimental results in the literature on organometallic compounds. Organometallic predictive methods have been developed for the following properties (reliability estimates are given in parentheses): ideal gas enthalpies of formation (2.3%), enthalpy of vaporization (4.8%), ideal gas heat capacity (4.0%), ideal gas entropy (1.3%), critical temperature (1.9%), critical pressure (4.7%), critical volume (6.2%), thermal conductivity (6.7%), and surface tension (6.2%).

Introduction

The increasing application of organometallic compounds in the specialty and commodity chemical industries has created a greater need for property data for these compounds by design engineers. Unfortunately, the number of experimental data in the literature for these compounds is sparse. When experimental data are difficult to obtain, data prediction methods become an invaluable alternative. Frequently organometallic compounds have been ignored in the development of data prediction methods. This paper presents the results of a project undertaken to develop methods for predicting thermodynamic and transport properties of organometallic compounds containing silicon, boron, and aluminum. These particular compounds were chosen, on the basis of their importance to industry, as well as the availability of experimental data needed to develop the prediction methods.

For organometallic compounds, the scarcity of experimental data on most properties has virtually eliminated the possibility of developing predictive methods that require data on other properties. For instance, a method to predict the thermal conductivity of a compound which requires viscosity and surface tension data is of little use if these data are not available. The difficulties incurred in obtaining experimental property data for these compounds have been partially overcome by the development of prediction techniques which are based on structure and which require little or no other experimental data. The literature contains a plethora of structural prediction methods that are applicable to organic compounds, but few give any treatment to organometallics. These methods, however, can be readily modified to include these compounds if sufficient experimental data are available. Except for thermal conductivity, the methods presented in this paper are all based on the structural contribution concept. The cited references for each method should be consulted for the specifics not related to organometallic compounds. Alternatively Danner and Daubert (*1*) present all the basic methods. The aspects of each method pertaining to organometallics are discussed in detail in this paper.

Structural Prediction Methods. Structural prediction methods are essentially based on three types of contributions: atomic, bond, or group. The chemical structure of a compound is required to identify the contributions contained in a compound. These contribution values are summed to determine a characteristic parameter which is then used in an equation to predict the desired property. For instance, a parachor is determined from atomic contributions, and this parameter is then used in an equation with the density to predict surface tension. Methods employing group contributions are typically the most accurate, but require a large data base to develop. Considerable effort was given to develop group contributions for all of the properties covered in this work. Unfortunately, an adequate number of experimental data were not available to do so. Since bond and atomic contribution methods require less data and are found to give reasonable results for some properties, these methods were used as appropriate.

Data Base. A comprehensive data base was generated in order to develop and evaluate the predictive methods. Over 200 references were consulted in order to obtain the most recent and reliable experimental data available. The complete data base, with references, is presented in the Appendix. The data are divided by property into separate tables each containing the experimental data for all of the compounds used to develop each predictive method. These tables also contain a compound by compound evaluation of the predictive methods covered.

Development of the Methods. The data bases for each of the seven properties of interest were used to evaluate any prediction methods currently available for organometallic compounds, to revise the methods when necessary, and to extend existing prediction methods that were not applicable to organometallic compounds.

For each of the structural methods, the group, bond, or atomic contributions were determined in the same general manner. The nonorganometallic contributions in an existing method were not redetermined; these values were used to isolate (by subtraction) the organometallic contribution values. The values for the organometallic contributions were determined by a series of stepwise nonlinear regressions. The contributions occurring most frequently in the organometallic compounds in the data base were determined first. Additional groups were added to the regression in order of decreasing frequency of occurrence. Some contributions were found to be present in only one compound, and could not be regressed. These contributions are noted in the tables; the reliability of predictions using them is questionable.

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Ideal Gas Enthalpies of Formation at 298.15 K

For ideal gas enthalpy of formation predictions, the group contribution technique developed by Benson et al. (2) has been shown to give reliable results for organic compounds. This method is applicable to certain organometallic compounds; however, it has been found to give results far less reliable than for other classes of organic compounds. This can be attributed to the scarcity and inaccuracy of data on organometallic compounds accessible to Benson and his coworkers when the method was developed. The quantity and quality of organometallic enthalpy of formation data have improved significantly, making it possible to refine this prediction method by determining new contribution values for silicon, boron, and aluminum compounds.

Group Contribution Method for $\Delta H^\circ_{f,298}$. Enthalpy of formation predictions by the Benson group contribution method require the use of the following equation:

$$\Delta H^\circ{}_{f,298} = \sum \nu_i \Delta H^\circ{}_{i,f,298} \qquad (1)$$

where $\Delta H^\circ{}_{f,298}$ is the enthalpy of formation of the ideal gas at 298.15 K. ν_i is the number of groups of type i, and $\Delta H^\circ{}_{i,f,298}$ is the type i group contribution. The group contributions for organometallic compounds are found in Table I. Contribution values for all nonorganometallic contribution are given by Benson et al. (2).

The Benson method requires the use of a correction factor to account for steric hinderences in a compound. These corrections, known as gauche corrections, are frequently required for branched compounds. Gauche corrections are only necessary for first-row elements. Benson attributed this to the greater bond lengths that occur with increasing molecular size. Hence, they are unnecessary for the second-row elements such as aluminum and silicon, although corrections for their substituents may be required. Boron being a first-row element requires the use of gauche corrections. Benson incorporated many of these corrections into the values of the groups. In the development of the new group contributions for boron compounds, gauche corrections were not combined with the group contribution values. This was done in order to avoid any confusion that may arise as to whether or not a gauche correction should be directly added to the sum of the group contributions in a heat of formation calculation. These corrections should always be accounted for explicitly.

Bond Contribution Method for $\Delta H^\circ_{f,298}$. The enthalpy of formation of some important silicon compounds, such as aminosilanes and silazanes, cannot be estimated using the group contribution method because of the lack of parameters for necessary groups. A sufficient number of data could not be obtained to determine these group contributions. A revised bond contribution method, based on a bond method also developed by Benson (3), was extended and is presented as an alternate procedure.

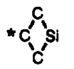
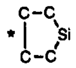
Enthalpy of formation predictions for silicon compounds by the bond contribution procedure require the following equation:

$$\Delta H^\circ{}_{f,298} = \sum \nu_i (\text{X--Y})_i \qquad (2)$$

where $\Delta H^\circ{}_{f,298}$ is the enthalpy of formation of the ideal gas at 298.15 K, ν_i is the number of X–Y bonds in the compound, and (X–Y)$_i$ is the bond contribution of atom X bonded to atom Y. The organometallic bond contribution values are given in Table II. Additional contributions can be obtained from Benson (3).

Evaluation and Comparison of the Methods for $\Delta H^\circ_{f,298}$. The group and bond contribution methods for enthalpy of formation predictions were evaluated against a data base containing experimental enthalpies of formation on 227 organometallic compounds. The group contribution method was evaluated by employing organometallic group contribution values from three sources: the new groups given in Table I, the groups given by Benson et al. (2), and groups developed by O'Neal and Ring (4).

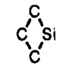
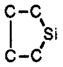
Table I. Group Contributions for the Prediction of the Enthalpy of Formation ($\Delta H^\circ_{f,298}$) at 298.15 K for Organometallic Compounds[a,b]

group	$\Delta H^\circ{}_{i,f,298}$/ (kJ mol^{-1})	group	$\Delta H^\circ{}_{i,f,298}$/ (kJ mol^{-1})
Si-(C)(H)$_3$	-39.4	C-(B)(C)$_2$(H)	4.7
Si-(C)$_2$(H)$_2$	-21.7	C-(B)(H)$_3$	-42.2
Si-(C)$_3$(H)	-38.6	B-(C$_B$)$_3$	-155.6
Si-(C)$_4$	-60.4	C$_B$-(B)	25.8
*Si-(Si)(H)$_3$	40.0	B-(O)$_3$	-279.5
*Si-(Si)$_2$(H)$_2$	40.9	B-(O)$_2$(H)	-150.4
Si-(Si)$_2$(C)$_2$	-18.3	*B-(O)(H)$_2$	-34.7
Si-(Si)(C)$_3$	-55.8	B-(B)$_2$(O)$_2$	-142.2
*Si-(Si)$_4$	169.9	O-(B)(C)	-170.9
C-(Si)(C)(H)$_2$	-17.3	O-(B)(H)	-255.7
C-(Si)(C)$_2$(H)	-2.2	O-(B)(C$_B$)	-173.6
C-(Si)(H)$_3$	-42.2	O-(B)(O)	-54.1
Si-(C)(Cl)$_3$	-487.2	*B-(C)$_2$(O)	-103.5
*Si-(C)$_2$(Cl)$_2$	-364.0	*B-(C$_B$)(O)$_2$	-218.5
*Si-(C)$_3$(Cl)	-227.3	B-(S)$_3$	-279.5
*Si-(C)(F)$_3$	-1190.5	S-(B)(C)	67.2
*Si-(C)$_3$(Br)	-166.7	*S-(B)(C$_B$)	88.1
*Si-(C)$_3$(I)	-80.4	B-(N)$_3$	-279.5
*Si-(C)(H)(Cl)$_2$	-359.8	B-(C)$_2$(N)	-131.3
*Si-(C)$_2$(H)(Cl)	-208.3	*B-(C)(N)(O)	-199.5
*Si-(O)(F)$_3$	-1274.0	N-(B)(C)$_2$	95.7
*Si-(O)$_3$(Cl)	-656.8	N-(B)(C)(H)	-126.0
*Si-(Si)(F)$_3$	-1183.0	*B-(O)(F)$_2$	-834.9
*Si-(Si)$_2$(F)$_2$	-795.7	*B-(O)$_2$(F)	-531.3
*Si-(Si)(Cl)$_3$	-493.2	*B-(B)(F)$_2$	-715.9
*Si-(Si)(O)$_3$	-238.3	B-(C)(F)$_2$	-806.2
Si-(O)$_3$(H)	-98.3	*B-(N)$_2$(Cl)	-357.5
Si-(C)(O)$_3$	-196.0	*B-(N)(Cl)$_2$	-412.7
Si-(C)$_2$(O)$_2$	-144.1	*B-(B)(Cl)$_2$	-244.6
Si-(C)$_3$(O)	-95.5	B-(O)$_2$(Cl)	-321.4
Si-(O)$_4$	-256.3	*B-(O)(Cl)$_2$	-374.7
*O-(Si)(O)	-91.4	*B-(C)$_2$(Cl)	-175.2
O-(Si)$_2$	-357.0	*B-(C$_B$)$_2$(Cl)	-283.2
O-(Si)(C)	-190.8	B-(C$_B$)(Cl)$_2$	-343.5
O-(Si)(H)	-283.1	B-(C)$_2$(Br)	-111.6
*Si-(Si)(C)(O)$_2$	-494.8	*B-(C$_B$)$_2$(Br)	-199.1
*C-(Si)(O)(H)$_2$	-7.8	*B-(C$_B$)(Br)$_2$	-224.2
*Si-(C$_B$)$_4$	-57.1	*B-(C)$_2$(I)	-35.8
*Si-(C$_B$)$_2$(Cl)$_2$	-404.3	Al-(C)$_3$	45.3
*Si-(C$_B$)(O)$_3$	-196.2	C-(Al)(C)(H)$_2$	-28.4
Si-(C$_B$)$_2$(C)(H)	-38.6	Al-(C)$_2$(H)	-9.0
C$_B$-(Si)	28.7	Al-(C)$_2$(Cl)	-265.2
O-(Si)(C$_B$)	-217.6	C-(Al)(H)$_3$	-42.2
B-(C)$_3$	3.7	*Al-(Al)(Cl)$_2$	-405.9
C-(B)(C)(H)$_2$	-13.2		
	Ring Corrections		
	62.9		41.2

[a] Group assignments are C-(Si)(H)$_3$ ≡ C-(B)(H)$_3$ ≡ C-(Al)(H)$_3$ ≡ C-(C)(H)$_3$, Si-(C$_B$)$_2$(C)(H) ≡ Si-(C)$_3$(H), and B-(O)$_3$ ≡ B-(N)$_3$ ≡ B-(S)$_3$ ≡ P-(O)$_3$. [b] An asterisk indicates a group determined by a single compound.

For silicon, the new groups produced predictions that were superior in accuracy and were applicable to a greater number of compounds than those given by O'Neal and Ring. The shortcomings of the O'Neal and Ring method can be attributed to the manner in which they had determined their silicon contribution values. Their group contributions were determined by a data base that consisted of enthalpy of formation data that were calculated by another method (5). In effect their group method is an estimation method based on another estimation method. The 43 new silicon group contributions,

Table II. Bond Contributions for the Prediction of the Enthalpy of Formation ($\Delta H^\circ_{f,298}$) at 298.15 K for Tetravalent Silicon Compounds[a]

bond	$(X\text{-}Y)_i$/ (kJ mol^{-1})	bond	$(X\text{-}Y)_i$/ (kJ mol^{-1})
(Si-N)	-53.1	*(Si-S)	87.2
(Si-C)	-9.3	(Si-F)	-403.7
(Si-H)	8.6	(Si-Cl)	-165.7
(Si-Si)	25.1	(Si-Br)	-103.9
(Si-O)	-218.8	(Si-I)	-27.6
(Si-C_{phenyl})	15.5		
	Ring Corrections		
	68.2		45.4

[a] An asterisk indicates a group determined by a single compound.

Table III. Evaluation Results of Prediction Methods for the Enthalpy of Formation at 298.15 K[a]

	silicon		boron		aluminum	
method	av % dev	% of compds	av % dev	% of compds	av % dev	% of compds
	Group Contributions					
Benson	N/A	N/A	5.3	57	6.2	44
O'Neal and Ring	5.4	37	N/A	N/A	N/A	N/A
New	1.9	84	4.8	100	2.1	100
	Bond Contributions					
O'Neal and Ring	17.3	86	N/A	N/A	N/A	N/A
New	5.7	88	N/A	N/A	N/A	N/A

[a] Compounds with applicable data: silicon, 148; boron, 20; aluminum, 9.

however, were determined solely from the experimental data of 124 silicon compounds. The original Benson et al. method did not contain any group contributions for silicon.

For boron, 40 group contributions were determined, and for aluminum, 6 groups were determined. These groups, which are given in Table I, were compared with the boron and aluminum groups given by Benson et al. (*2*) by comparing the predicted values given by each method with the literature values given in the data base. Table III contains a summary of results. Improvements in the reliability and applicability of the method were realized from the new group values.

A comparison of the boron and aluminum contribution values developed by Benson et al. with those given in Table I will, in some instances, reveal large differences. In addition to the expected variations in group values associated with differences in the experimental data used in the regression, the greater quantity of data allowed for eliminating and changing some of the group assignments made by Benson et al. (*2*). This had a significant effect on group values overall.

Table II contains 11 silicon contribution values for use with the Benson bond contribution method. These values were determined from the experimental data of 131 silicon compounds. Similar work was originally done by O'Neal and Ring (*6*). A comparison between the new bond contribution values given in Table II and those recommended by O'Neal and Ring was accomplished by comparing the predicted values with the literature values for each compound in the data base. Greater accuracy was obtained with the new silicon bond contribution values. The large errors given by the O'Neal and Ring contributions are the results of their use of data from old and less reliable sources.

A compound by compound evaluation of the predictive methods discussed in this section is presented for 148 silicon compounds in Appendix Table A.1. Similarly, Table A.2 contains an evaluation for 79 boron and aluminum compounds. The percent deviation is defined in terms of the absolute difference as $100\{|H_{exptl} - H_{calcd}|/|H_{exptl}|\}$.

Sample Calculation. Sample calculations are given below to illustrate the use of the group (second-order) and bond (first-order) contribution methods. A prediction of the ideal gas enthalpy of formation of triethylsilane [$(C_2H_5)_3SiH$] is shown using each of these methods.

Group Contribution Method

group contribution	no. of groups	$\nu_i \Delta H^\circ_{i,f,298}$/(kJ mol^{-1})
Si-(C)$_3$(H)	1	1 (-38.6)
C-(Si)(C)(H)$_2$	3	3 (-17.3)
C-(C)(H)$_3$	3	3 (-42.2)
		$\Delta H^\circ_{f,298} = -217.1$ kJ mol^{-1}

Bond Contribution Method

bond contribution	no. of bonds	$\nu_i(X\text{-}Y)_i$/(kJ mol^{-1})
Si–C	3	3 (-9.3)
Si–H	1	1 (8.6)
C–C	3	3 (11.4)
C–H	15	15 (-16.0)
		$\Delta H^\circ_{f,298} = -225.1$ kJ mol^{-1}

An experimental value of −216.5 kJ mol^{-1} is given by Voronkov et al. (*7*).

Enthalpy of Vaporization

A group contribution method for the prediction of enthalpies of vaporization at 298.15 K has been evaluated and subsequently modified for use with organometallic compounds. This method, originally developed by Ducros et al. (*8–11*), is unique among prediction methods currently available for this property. A majority of enthalpy of vaporization methods are based on corresponding states, which require critical property input data that are not readily available for organometallic compounds. The group contribution method, however, only requires a chemical structure, and is therefore very appropriate for predictions of this property for organometallic compounds.

In order to evaluate the group contribution method as presented by Ducros et al., reported experimental enthalpy of vaporization data at 298.15 K were collected from the literature for organometallic compounds containing silicon, boron, and aluminum. Poor results were obtained in the evaluation, suggesting the need to revise the organometallic group contribution values. These results can be attributed to the fact that only some of the experimental data available for these compounds were utilized in the original development of the organometallic contribution values.

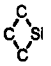
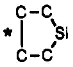
An additional enthalpy of vaporization prediction technique for organic compounds requiring an acentric factor and reduced temperature developed by Katinas and Danner (*12*) has been evaluated and is presented as an alternative to the group contribution method for organosilicon compounds. Since critical property data are not readily attainable for boron and aluminum compounds, and predictive methods are also somewhat restricted, this method could not be evaluated for these compounds.

Group Contribution Method for $\Delta H^\circ_{v,298}$. Predictions of the enthalpy of vaporization for organometallic compounds at 298.15 K by the revised Ducros et al. group contribution method require the group contributions given in Table IV and the following equation:

$$\Delta H_{v,298} = \sum \nu_i \Delta H_{i,v,298} \quad (3)$$

Here $\Delta H_{v,298}$ is the enthalpy of vaporization at 298.15 K, ν_i is the number of groups of type i, and $\Delta H_{i,v,298}$ is the type i group contribution. The method requires additional group

Table IV. Group Contributions for the Prediction of the Enthalpy of Formation ($\Delta H_{v,298}$) at 298.15 K for Organometallic Compounds[a,b]

group	$\Delta H_{i,v,298}$/ (kJ mol^{-1})	group	$\Delta H_{i,v,298}$/ (kJ mol^{-1})
$Si-(C)(H)_3$	18.74	$N-(Si)(C)(H)$	10.13
$Si-(C)_2(H)_2$	11.65	$N-(Si)(C)_2$	1.12
$Si-(C)_3(H)$	11.17	$N-(Si)_2(C)$	-7.19
$Si-(C)_4$	10.85	$Si-(N)(C)(H)_2$	10.13
$C-(Si)(C)(H)_2$	1.89	* $N-(Si)_2(H)$	0.96
$C-(Si)(C)_2(H)$	-1.94	* $Si-(N)_3(H)$	13.30
$C-(Si)(H)_3$	5.65	* $N-(Si)_3$	-6.26
$C_{Si}-(C)_2(H)_2$	1.43	$B-(C)_3$	3.27
$C_{Si}-(C)_3(H)$	-3.35	$C-(B)(C)(H)_2$	3.12
$C_{Si}-(O)(C)(H)_2$	1.71	$C-(B)(C)_2(H)$	1.57
* $C_{Si}-(O)(C)_2(H)$	-10.19	$C-(B)(H)_3$	5.65
$Si-(Si)(C)_3$	1.94	$O-(B)(C)$	4.23
$C-(Si)_2(C)_2$	-3.85	$B-(O)(C)_2$	8.88
* $Si-(Si)_4$	-22.40	$B-(O)_2(C)$	3.99
$Si-(O)(C)_3$	6.08	$O-(B)(H)$	14.10
$O-(Si)_2$	-9.19	* $B-(B)(C)_2$	4.40
$Si-(O)_2(C)_2$	2.94	$B-(B)(O)_2$	2.49
$Si-(O)_3(C)$	-2.55	$B-(S)_3$	5.06
$O-(Si)(C)$	5.69	$S-(B)(C)$	11.35
* $O-(Si)(H)$	22.52	*$B-(C)_2(Cl)$	12.29
$Si-(O)_4$	-6.86	$B-(O)_2(Cl)$	12.24
$Si-(Si)(H)_3$	9.37	$B-(O)(Cl)_2$	21.27
$Si-(Si)_2(H)_2$	10.20	$B-(C)(Cl)_2$	18.20
$Si-(O)(C)_2(Cl)$	16.27	*$B-(B)(Cl)_2$	15.50
*$Si-(Si)(F)_3$	13.60	$B-(C)_2(Br)$	21.67
*$Si-(Si)_2(F)_2$	9.60	*$B-(C)_2(I)$	17.14
$Si-(C)(F)_3$	14.87	*$B-(C)(Br)_2$	29.11
$Si-(C)_2(F)_2$	14.89	*$B-(N)_3$	-0.95
*$Si-(C)_3(F)$	25.35	*$N-(B)(C)2$	4.65
$Si-(C)(Cl)_3$	28.31	*$B-(B)(N)_2$	-4.60
$Si-(C)(Cl)_2(H)$	22.98	$B-(N)(C)_2$	4.65
$Si-(C)_2(Cl)_2$	25.53	*$B-(O)(N)(C)$	10.96
*$Si-(C)_2(Cl)(H)$	17.20	*$N-(B)(C)(H)$	31.53
$Si-(C)_3(Cl)$	15.32	*$B-(N)_2(H)$	6.80
$Si-(C)(Cl)_2(F)$	23.41	*$B-(N)_2(F)$	6.90
$Si-(C)(Cl)(F)_2$	20.03	$B-(N)(Cl)_2$	22.16
*$Si-(C)(Cl)(F)(H)$	23.65	*$B-(N)_2(Cl)$	9.90
*$Si-(C)_2(Cl)(F)$	17.10	$C_B-(B)(C_B)_2$	-13.40
*$Si-(C)_3(Br)$	15.65	$C_d-(B)(C_d)(H)$	5.29
*$Si-(C)(H)_2(Br)$	22.85	$Al-(C)_3$	46.55
$Si-(O)(Cl)_3$	24.76	$C-(Al)(C)(H)_2$	3.29
*$Si-(O)(C)(Cl)_2$	15.01	$C-(Al)(H)_3$	5.65
$Si-(Si)(Cl)_3$	23.45	* $Al-(C)_2(H)$	34.17
$C_B-(Si)(C_B)_2$	-6.48	$Al-(C)_2(O)$	12.82
$C_d-(Si)(C_d)(H)$	3.37	$O-(Al)(C)$	4.23
$C-(Si)(C_d)(H)_2$	0.18	*$Al-(C)_2(Cl)$	11.90
$Si-(N)(C)_3$	3.27		
	Ring Corrections		
* 	7.34	* 	8.91

[a] Group assignments are $C-(Si)(H)_3 \equiv C-(B)(H)_3 \equiv C-(Al)(H)_3 \equiv C-(C)(H)_3$, $Si-(N)(C)(H)_2 \equiv N-(Si)(C)(H)$, $N-(B)(C)_2 \equiv B-(N)(C)_2$, $B-(S)_3 \equiv N-(C)_3$, and $O-(Al)(C) \equiv O-(B)(C)$. [b] An asterisk indicates a group determined by a single compound.

contributions that are not presented here; these can be obtained from Ducros et al. (*8–11*).

Two modifications of the Ducros et al. method for organometallic compound predictions were made. First, separate carbon–hydrogen contributions were developed to be used exclusively with alkyl and alkoxy silicon compounds. These special group values are designated by an Si subscript on the group and are to be used only when a silicon compound is exclusively made up of alkyl or alkoxy substituents. When a compound contains halogens, nitrogen, and other non-alkyl or non-alkoxy substituents, the standard group contributions are to be used. Boron and aluminum compounds do not require these special groups. Second, central organometallic group contributions involving double-bonded or aromatic carbons are equal to the contributions that had only single-bonded carbons. For instance, the groups $Si-(C_B)_2(C)_2$ and $Si-(C)_4$ have the same contribution value.

Table V. Evaluation Results of Prediction Methods for the Enthalpy of Vaporization at 298.15 K[a]

	silicon		boron	
method	av % dev	% of compds	av % dev	% of compds
New Groups	5.3	100	3.4	100
Acentric Factor	8.3	37	N/A	N/A

[a] Compounds with applicable data: silicon,151; boron,52.

Acentric Factor Prediction Method for $\Delta H_{v,298}$. The acentric factor method for the enthalpy of vaporization is given in complete detail by Katinas and Danner (*12*). To apply this method, an acentric factor and critical temperature of a compound must be obtained. These properties are required in order to determine a dimensionless enthalpy of vaporization ($\Delta H_v M/RT_c$). This dimensionless parameter is given as a function of the reduced temperature (T_r) and the acentric factor. If experimental critical property data cannot be obtained, they can be predicted by methods presented in this paper. This method is applicable to temperatures other than 298.15 K; however, it was evaluated using an enthalpy of vaporization data base containing data only at 298.15 K. Consequently, the expected reliability at other temperatures is not known.

Evaluation of the Methods for $\Delta H_{v,298}$. The modifications and revisions of the Ducros et al. group contribution method, for organometallics, have resulted in a significantly improved means of predicting the enthalpy of vaporization for these compounds. A total of 93 organometallic group contributions were developed from the experimental data of 211 compounds. This represents a significant improvement in the number of groups available when compared to that of Ducros et al. who have reported 52 such groups. The regression of new contribution values has also greatly improved the reliability of this method. This is borne out by the results of a comparison of predicted data against literature values given in Table V. Only eight compounds were available for the determination of the aluminum group contributions. The resulting deviations were very small except for $HAl(i\text{-}C_4H_9)_2$. (See Appendix Table A.4) The acentric factor method was also evaluated to predict $\Delta H_{v,298}$ but only for the silicon compounds. When compared against experimental data, the method gave an average error of 8.3% and a percent bias of +6.1%. The percent bias indicates that this method has a tendency to overpredict. The method could not be used to predict the enthalpy of vaporization for all silicon compounds in the data base because of limitations in vapor pressure data and the applicability of the critical property predictions. A complete evaluation of the group contribution method and acentric factor method is given in Appendix Tables A.3 and A.4.

The revised group contribution method of Ducros et al. is recommended as the primary method for enthalpy of vaporization predictions at 298.15 K for organometallic compounds containing silicon, boron, and aluminum. This method has been proven to be more applicable for a greater number of compounds and has been shown to be more accurate than the acentric factor method. The acentric factor method should be used for silicon compounds only if the group contribution method cannot be applied. The reliability of this method has been verified at 298 K only; therefore, strict judgements on its applicability at other temperatures cannot be made.

Table VI. Atomic Contributions ($\theta_{i,T}$) for the Prediction of the Heat Capacity ($C°_p$) for Organometallic Compounds

	$\theta_{i,T}$/(J mol^{-1} K^{-1})		
T/K	Si	Al	B
300	17.5	16.6	10.5
400	19.8	19.1	13.7
500	22.3	21.0	16.1
600	22.1	22.5	17.8
800	24.5	24.0	20.5
1000	24.6	24.5	21.6
1500	24.0	25.0	22.7

Heat Capacity Prediction Methods

A zero-order atomic contribution technique for isobaric ideal gas heat capacity estimations of various organic and inorganic compounds, developed by Harrison and Seaton (*13*), has been revised by redetermining contribution values for silicon, boron, and aluminum. This procedure predicts C_p at seven temperatures between 300 and 1500 K for a wide range of organic and organometallic compounds. A data base consisting of over 900 experimental values was obtained in order to develop the 21 new contribution values and to evaluate the reliability of this method in its original and revised forms.

The compound under consideration is decomposed into its constituent atoms. The ideal gas heat capacity is then estimated by the summation of a constant and the individual heat capacity atomic contributions as in the following equation:

$$C°_{p,T} = K_T + \sum \nu_i \theta_{i,T} \qquad (4)$$

Here $C°_{p,T}$ is the isobaric ideal gas heat capacity at a temperature T, K_T is a constant at temperature T, ν_i is the number of atoms of type i, and $\theta_{i,T}$ is the atomic contribution of the atom at temperature T. The atomic contribution values for silicon, boron, and aluminum are listed in Table VI for seven temperatures between 300 and 1500 K. Additional contributions are given by Harrison and Seaton (*13*). When a prediction is required at a temperature other than those listed, Harrison and Seaton recommend a linear interpolation between the listed temperatures.

Harrison and Seaton have suggested that their atomic contribution method is capable of being used in conjunction with group contribution methods. They claim that the method will provide suitable values for any missing group contribution that is required in a prediction. This is done by building a molecule which contains the group contribution that is desired, as well as contributions whose values are readily available. The heat capacity of this molecule is then predicted by the atomic contribution method. The group contribution values that are known are then subtracted from the predicted $C°_p$ value, leaving the contribution of the unknown group. This value can then be used to predict the ideal heat capacity of other molecules. This kind of approach would result in a hybrid of the methods with an accuracy that lies somewhere between the two, but retaining the wide range of applicability of atomic contribution methods.

The contribution values for silicon, boron, and aluminum developed by Harrison and Seaton were compared against the revised contribution values given in Table VI. Predictions for both methods were computed and compared against a data base containing over 900 experimental values spanning a temperature range of 300–1500 K. A summary of results is given in Table VII. A detailed evaluation of the method using the revised contribution values is presented in Table A.5 in the Appendix. Modest improvements were realized.

Table VII. Evaluation Results of Prediction Methods for the Ideal Gas Heat Capacity[a]

method	silicon av % dev	boron av % dev	aluminum av % dev
Original	4.2	4.4	5.8
Revised	3.8	3.7	5.4

[a] Data points used: silicon, 458; boron, 298; aluminum, 148.

Table VIII. Extended Benson Bond Contributions for Ideal Gas Entropy Predictions at 298.15 K[a]

Bond	(X–Y)$_i$/ (J mol^{-1} K^{-1})	bond	(X–Y)$_i$/ (J mol^{-1} K^{-1})
(Si-C)	-58.47	*(Si-C≡N)	104.30
(Si-C$_{\text{phenyl}}$)	109.10	*(Si-N=C=S)	147.90
(Si-Si)	-47.98	(B-C)	-42.38
(Si-O)	-29.27	(B-O)	-5.90
(Si-H)	57.05	(B-B)	-20.08
(Si-F)	76.89	(B-H)	67.60
(Si-Cl)	89.15	(B-F)	88.49
(Si-Br)	99.71	(B-Cl)	99.55
* (Si-I)	109.04	(B-Br)	112.86
*(Si-C≡CH)	107.40		

[a] Asterisk indicates a group determined by a single compound.

Table IX. Evaluation Results of Prediction Methods for the Ideal Gas Entropy at 298.15 K[a]

	silicon		boron	
	av % dev	% of compds	av % dev	% of compds
van Dalen and van den Berg	0.6	27	N/A	N/A
O'Neal and Ring	1.1	71	N/A	N/A
New	1.3	100	1.1	100

[a] Compounds with applicable data: silicon, 68; boron, 20.

Ideal Gas Entropies at 298.15 K

A procedure for predicting ideal gas entropies at 298.15 K has been developed for use with silicon and boron compounds. This prediction scheme is an extension of a bond contribution method developed by Benson (*3*). For silicon, 12 bond contribution values were determined from the experimental entropy data of 68 compounds, and for boron, 7 bond values were determined from 20 compounds. Unfortunately, sufficient experimental data to determine aluminum contribution values were not available.

The bond contribution procedure will predict the ideal gas entropy at 298.15 K of pure silicon and boron compounds. The method requires the use of the bond contribution values given in Table VIII and the equation given below:

$$S°_{298} = \sum \nu_i (\text{X–Y})_i - R \ln \phi \qquad (5)$$

Here $S°_{298}$ is the entropy of the compound, $(\text{X–Y})_i$ is the bond contribution of atom X bonded to Y, ν_i is the number of $(\text{X–Y})_i$ bonds in the compound, R is the gas constant, and ϕ is the symmetry number. Additional bond contributions are given by Benson (*3*).

The new bond contribution method was compared with two similar prediction methods for silicon compounds developed by O'Neal and Ring (*6*) and by van Dalen and van den Burg (*14*). The complete results of the evaluation of these methods against experimental data values for 68 silicon compounds are presented in Appendix Table A.6. Table A.7 contains an evaluation of the new contribution method for 20 boron compounds. Table IX contains a summary of these results. For silicon compounds the reliability of these three methods is very similar. The new contribution method is applicable to a greater number of silicon compounds, however, than the other methods and gives more accurate predictions when it is directly compared for the same limited number of compounds. In addition, only the new contribution method contains values for boron compounds.

Critical Properties

Structural contribution methods for critical property predictions have been enhanced for application to silicon-containing compounds. These predictive schemes have been amended by either revising existing silicon contribution values or developing new silicon contributions that were previously unavailable. These modifications were possible because of the existence of a more comprehensive and reliable silicon critical property data base. Sufficient experimental data on critical properties were not available to develop methods for boron and aluminum compounds.

A data base consisting of critical temperature and pressure data was employed to regress silicon contribution values for use with the prediction methods developed by Lyderson (*15*) and Ambrose (*16*, *17*). For critical temperature, 5 silicon contribution values for each method were determined from the experimental data of 45 compounds. Similarly, 4 contribution values for critical pressure were determined from 31 compounds. The Lyderson and Ambrose methods were selected because of their simplicity and reliability. For critical volume predictions, the Fedors method (*18*) was extended to include silicon compounds. This method was modified by regressing three contribution values for silicon from a data base consisting of 31 compounds. The Fedors method was chosen over more elaborate prediction methods for two reasons. First, the amount of experimental data available was limited. Second, critical volume measurements tend to be imprecise.

The most significant modification to the predictive methods discussed above was the development of separate silicon contribution values for siloxane compounds. These values were regressed independently of the other silicon contributions. As a result, all contributions were subsequently made more reliable. The original Ambrose prediction methods for critical temperature and pressure were not evaluated, since they were applicable to only a limited number of silicon compounds.

Critical Temperature. Critical temperature predictions employing the Lyderson method require the following equation:

$$T_c/\mathrm{K} = \frac{T_b/\mathrm{K}}{[0.567 + \sum \Delta_T - (\sum \Delta_T)^2]} \qquad (6)$$

Here T_c and T_b are the critical and boiling temperatures, respectively. $\sum\Delta_T$ is the sum over all groups present of the Lyderson critical temperature contributions. The Ambrose method uses the following equation:

$$\frac{T_b}{T_c - T_b} = 1.242 + \sum \Delta_T{}^\circ \qquad (7)$$

where T_c and T_b are the critical and boiling temperatures, respectively. $\sum\Delta_T{}^\circ$ is the sum over all groups in the molecule of the Ambrose group contributions.

Critical Pressure. The Lyderson prediction method for critical pressures requires the following equation:

$$P_c/\mathrm{MPa} = \frac{0.101325M}{[0.34 + (\sum \Delta_P)]^2} \qquad (8)$$

Here P_c is the critical pressure of a compound, M is the molecular weight, and $\sum\Delta_P$ is the sum of the Lyderson critical pressure group contributions.

Table X. Group and Atomic Contributions for Critical Property Prediction Methods

Critical Temperature

Lyderson	Δ_T	Ambrose	$\Delta^\circ{}_T$
$-\overset{\vert}{\underset{\vert}{Si}}-$	0.026	$-\overset{\vert}{\underset{\vert}{Si}}-$	0.138
$-\overset{\vert}{\underset{\vert}{Si}}H$	0.040	$-\overset{\vert}{\underset{\vert}{Si}}H$	0.371
$-SiH_3$	0.027	$-SiH_3$	0.195
$-\overset{\vert}{\underset{\vert}{Si}}-O-$	0.025	$-\overset{\vert}{\underset{\vert}{Si}}-O-$	0.159
$[-\overset{\vert}{\underset{\vert}{Si}}-O-]_{cyclic}$	0.027	$[-\overset{\vert}{\underset{\vert}{Si}}-O-]_{cyclic}$	0.131

Critical Pressure

Lyderson	Δ_P	Ambrose	$\Delta^\circ{}_P$
$-\overset{\vert}{\underset{\vert}{Si}}-$	0.468	$-\overset{\vert}{\underset{\vert}{Si}}-$	0.0461
$-\overset{\vert}{\underset{\vert}{Si}}H$	0.513	$-\overset{\vert}{\underset{\vert}{Si}}H$	0.0507
$-\overset{\vert}{\underset{\vert}{Si}}-O-$	0.730	$-\overset{\vert}{\underset{\vert}{Si}}-O-$	0.0725
$[-\overset{\vert}{\underset{\vert}{Si}}-O-]_{cyclic}$	0.668	$[-\overset{\vert}{\underset{\vert}{Si}}-O-]_{cyclic}$	0.0663

Critical Volume

Fedor	Δ_V
Si	0.086174
$Si_{siloxane}$	0.126483
$Si_{cyclic\ siloxane}$	0.094576

The Ambrose method is recommended by Danner and Daubert (*1*) as an alternative to the Lyderson method, particularly for alcohols, ketones, mercaptans, and sulfides. Predictions are made by the following equation:

$$P_c/\mathrm{MPa} = \frac{10^{-3}M}{[0.0339 + (\sum \Delta_P{}^\circ)]^2} \qquad (9)$$

Here P_c is the critical pressure of a compound, M is the molecular weight, and $\sum\Delta_P{}^\circ$ is the sum of the group contributions determined by Ambrose.

Critical Volume. The method of Fedors for critical volume predictions requires the following equation:

$$V_c/(\mathrm{m^3\,kmol^{-1}}) = 0.0266 + \sum \Delta_V \qquad (10)$$

Here V_c is the critical volume of a compound and $\sum\Delta_V$ is the sum over all groups of the Fedors atomic contributions.

The new silicon contribution values regressed for the above methods are listed in Table X. Additional contributions can be obtained from the original references or from Danner and Daubert (*1*). The improvements in accuracy and in versatility attained by revising and determining new silicon contribution values for critical property predictions are borne out by the evaluation results presented in Table XI. Critical temperature predictions by the Lyderson method have been improved by almost 1% overall and by over 1.5% for siloxanes. The extended Ambrose method gave less accurate results. Only

Table XI. Evaluation Results of Prediction Methods for Critical Properties[a]

	T_c		P_c		V_c	
method	av % dev	% of compds	av % dev	% of compds	av % dev	% of compds
			Overall			
Lyderson	2.68	88	4.94	93	N/A	N/A
Rev. Lyderson	1.92	100	4.66	100	N/A	N/A
Ext. Ambrose	3.10	100	4.76	100	N/A	N/A
Fedor	N/A	N/A	N/A	N/A	6.17	100
			Siloxanes			
Lyderson	3.50	90	1.87	90	N/A	N/A
Rev. Lyderson	1.98	100	1.59	100	N/A	N/A
Ext. Ambrose	2.72	100	1.62	100	N/A	N/A
Fedor	N/A	N/A	N/A	N/A	3.90	100

[a] Compounds with applicable data: (overall) T_c, 43; P_c, 27; V_c, 31; (siloxanes) T_c, 27; P_c, 10; V_c, 12.

slight improvements were made in the Lyderson method for critical pressures, because of the relatively modest size of the critical pressure data base which contained data for only 27 silicon compounds. The extended Ambrose method for critical pressures gave similar results. Critical volume predictions by the Fedors method were compared against literature values for 31 silicon compounds. An average deviation of 6.17% was obtained. This lower overall accuracy is a reflection of the decreased reliability of the experimental data for critical volumes. The complete critical property data base and detailed evaluations of the predictive methods discussed are presented in Appendix Tables A.8–A.10.

Liquid Thermal Conductivity

An estimation technique for liquid thermal conductivities, based on a scheme devised by Baroncini et al. (*19*), has been developed for application to specific organosilicon compounds. This method was chosen because of its simplicity and accuracy of predictions for silicon compounds. Experimental thermal conductivity data were obtained from a literature search and used to regress correlative prediction formulas for (chloroalkyl)- and alkoxysilanes. The (chloroalkyl)silane prediction formula was determined from the data of 18 compounds. Similarly, the alkoxysilane formula was determined from 19 compounds. Unfortunately, additional formulas for other silicon compound classes could not be developed because experimental data for these compounds are virtually nonexistent.

These prediction formulas typically require the critical and boiling temperatures of a compound in addition to a molecular weight. If the critical temperature is not available, the predictive methods for critical temperature presented previously must be used.

The prediction equations for thermal conductivity of silicon compounds at various temperatures are presented below:

alkoxysilanes

$$k/(\mathrm{W\ m^{-1}\ K^{-1}}) = 0.00482\frac{(T_b/K)^{6/5}}{M^{1/2}(T_c/K)^{1/6}}\,\frac{(1-T_r)^{0.38}}{T_r^{1/6}} \tag{11}$$

(chloroalkyl(aryl))silanes

$$k/(\mathrm{W\ m^{-1}\ K^{-1}}) = 0.6510\frac{(T_b/K)^{6/5}}{M^{1/2}}\,\frac{(1-T_r)^{0.38}}{T_r^{1/6}} \tag{12}$$

Here k is the thermal conductivity of a liquid at a temperature T, T_b is the boiling temperature, T_c is the critical temperature, T_r is the reduced temperature, T/T_c, and M is the molecular weight of the compound. Poor results will be obtained if the predictive formulas, given above, are applied to silicon compounds other than those for which they were intended.

Table XII. Evaluation Results of the Correlative Prediction Formulas for the Liquid Thermal Conductivity of Silicon Compounds

compound class	av % dev	no. of compds	no. of data points
Alkoxysilanes	7.2	19	150
Chloroalkyl-(aryl)-silanes	6.2	18	18

Table XIII. Atomic Parachors ($\mathbf{P}_i$)/(mN$^{1/4}$ m$^{11/4}$ kmol^{-1}) for Organometallic Compounds

Si	30.3	B	13.2
$\mathrm{Si_{Silanes}}$	43.3	Al	34.9

Thermal conductivity data predicted by the Baroncini method were compared with the experimental values for all of the silicon compounds in the data base. A summary of results is given in Table XII. The complete evaluation is given in Appendix Table A.11. For 37 silicon compounds, the method gave predictions with a combined average deviation of approximately 7%.

Surface Tension

A method for estimating surface tensions has been refined for application to organometallic compounds. The method is based on the combined work of Macleod (*20*) and Sugden (*21*). Macleod has proposed a functional relationship among the surface tension, density, and parachor of a compound. The parachor is a temperature-independent constant, characteristic of a compound. Sugden had developed an atomic contribution method to predict this parameter. The combination of these ideas results in a surface tension prediction method that requires only the density and chemical formula. By employing a data base consisting of experimental data for surface tension and density on 100 organometallic compounds, contribution values for silicon, boron, and aluminum were regressed for parachor predictions. Regression of a single contribution for all silicon compounds gave poor results. Therefore, a special contribution value was developed to be used exclusively with silanes of the form $\mathrm{Si}_X\mathrm{H}_{2X-1}$. Since atomic contribution methods are applicable to most chemical compounds, and density data are easily obtained or measured, this prediction method is well suited for organometallic applications.

Predictions of surface tension require the contribution values given in Table XIII. The equation below is used to predict the parachor, $\mathbf{P}$, which is used along with the density to predict the surface tension. The density and surface tension predictions are at the same temperature:

$$\mathbf{P} = \sum \nu_i \mathbf{P}_i \tag{13}$$

where ν_i is the number of contributions of type i, and $\mathbf{P}_i$ is the atomic or structural contribution value of i to the parachor.

$$\sigma/(\mathrm{mN\ m^{-1}}) = [(\mathbf{P}/1000)\rho_L]^4 \tag{14}$$

Here σ is the surface tension, $\mathbf{P}$ is the parachor (mN$^{1/4}$ m$^{11/4}$ kmol^{-1}), and ρ_L is the liquid density at the temperature of interest (kmol m^{-3}).

The parachor prediction method for silicon, boron, and aluminum compounds predicts the parachor of a compound with a high degree of accuracy. The average percentage deviation for predicting parachors was 1.6%. When these predicted parachors were used with density data to predict the surface tension of the compounds in the data base, an

Table XIV. Evaluation Results of the Parachor Prediction Method for Surface Tensions

Si		B		Al	
av % dev	no. of compds	av % dev	no. of compds	av % dev	no. of compds
6.2	96	5.8	21	11.1	3

overall deviation of 6.2% was obtained as shown in Table XIV. The small deviations in predicted parachors are magnified when surface tensions are estimated. These results were obtained from the complete evaluation given in Appendix Table A.12.

Conclusions

Thermodynamic and transport property prediction methods have been developed for organometallic compounds, creating a valuable supplement to the prediction methods currently available in the literature. These methods, with the modifications presented here, are believed to be the most reliable and complete prediction methods available for silicon, boron, and aluminum compounds.

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Literature Cited

(1) Danner, R. P.; Daubert, T. E. *Data Prediction Manual*; Design Institute for Physical Property Data, American Institute of Chemical Engineers: New York, extant 1987.
(2) Benson, S. W.; Cruickshank, F. R.; Golden, D. M.; Haugen, G. R.; O'Neal, H. E.; Rodgers, A. S.; Shaw, R.; Walsh, R. *Chem. Rev.* **1969**, *69*, 279.
(3) Benson, S. W. *Thermochemical Kinetics*, 2nd ed.; John Wiley and Sons Inc.: New York, 1976.
(4) O'Neal, H. E.; Ring, M. A. *J. Organomet. Chem.* **1981**, *213*, 419.
(5) Benson, S. W. *Angew. Chem., Int. Ed. Engl.* **1978**, *17*, 812.
(6) O'Neal, H. E.; Ring, M. A. *Inorg. Chem.* **1966**, *5*, 435.
(7) Voronkov, M. G.; Baryshok, V. P.; Klyuchnikov, V. A.; Danilova, T. F.; Pepekin, V. I.; Korchagina, A. N.; Khudobin, Y. I. *J. Organomet. Chem.* **1988**, *345*, 27.
(8) Ducros, M.; Gruson, J. F.; Sannier, H. *Thermochim. Acta* **1980**, *36*, 39.
(9) Ducros, M.; Gruson, J. F.; Sannier, H. *Thermochim. Acta* **1981**, *44*, 131.
(10) Ducros, M.; Sannier, H. *Thermochim. Acta* **1982**, *54*, 153.
(11) Ducros, M.; Sannier, H. *Thermochim. Acta* **1984**, *75*, 329.
(12) Katinas, T. G.; Danner, R. P. *Hydrocarbon Process.* **1977**, *56* (3), 157.
(13) Harrison, K. B.; Seaton, W. H. *Ind. Eng. Chem. Res.* **1988**, *27*, 1536.
(14) van Dalan, M. J.; van den Berg, P. J. *J. Organomet. Chem.* **1970**, *24*, 277.
(15) Lyderson, A. L. Engineering Experimental Station Report 3; College of Engineering University of Wisconsin: Madison, WI, 1955.
(16) Ambrose, D. *Natl. Phys. Lab. Rep. Chem.* **1978**, *92*.
(17) Ambrose, D. *Natl. Phys. Lab. Rep. Chem.* **1979**, *98*.
(18) Fedors, R. F. *AIChE J.* **1979**, *25*, 202.
(19) Baroncini, C.; Di Filippo, P.; Latini, G.; Pacetti, M. *Int. J. Thermophys.* **1981**, *2*, 21.
(20) Macleod, D. B. *Trans. Faraday Soc.* **1923**, *19*, 38.
(21) Sugden, S. *J. Chem. Soc.* **1924**, *125*, 1177.

Appendix

This Appendix contains the complete data base used to develop and evaluate the new organometallic predictive methods. The data base is the culmination of an extensive literature search for experimental data. The data are divided into 12 tables, primarily by property.

For each compound, reference numbers are listed denoting the sources of the experimental data. These reference numbers refer to the references listed under Data References following the Appendix rather than those listed under Literature Cited. For most compounds more than one data reference is indicated. For these compounds each of the data references was critically evaluated in order to select the ones providing the most reliable data values. These references are underlined in the tables.

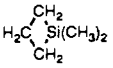
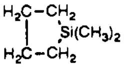
Table A.1. Predictions of the Standard Ideal Gas Enthalpy of Formation at 298.15 K for Silicon Compounds[a,b]

		new group contribution		O'Neal and Ring group contribution		new bond contribution		O'Neal and Ring bond contribution		
compound	exptl $-\Delta H^\circ_f$	$-\Delta H^\circ_f$	% dev	$-\Delta H^\circ_f$	% dev	$-\Delta H^\circ_f$	% dev	$-\Delta H_f$	% dev	ref
$(CH_3)_3SiH$	163.4	165.1	1.0	175.3	7.3	163.3	0.1	212.3	29.9	45, 66, 141, 170, 181, 182
$(C_2H_5)_3SiH$	216.5	217.1	0.2	214.0	1.2	225.1	4.0	273.9	26.5	141, 142, 143, 182, 188
$(C_3H_7)_3SiH$	280.0	279.1	0.3	275.9	1.5	286.9	2.5	335.7	19.9	188
$(C_4H_9)_3SiH$	341.0	341.3	0.1	337.8	0.9	348.7	2.3	397.5	16.6	188
$(C_5H_{11})_3SiH$	402.0	403.4	0.3	399.7	0.6	410.5	2.1	459.3	14.3	188
$(C_6H_{13})_3SiH$	466.0	465.5	0.1	461.6	1.0	472.3	1.4	521.1	11.8	188
$(C_7H_{15})_3SiH$	529.0	527.7	0.2	523.5	1.1	534.1	1.0	582.9	10.2	188
$(C_8H_{17})_3SiH$	591.0	589.8	0.2	585.4	1.0	595.9	0.8	644.7	9.1	188
$(C_9H_{19})_3SiH$	651.0	651.9	0.1	647.2	0.6	657.7	1.0	706.5	8.5	188
$(C_{10}H_{21})_3SiH$	713.0	714.0	0.1	709.1	0.5	719.5	0.9	768.3	7.8	188
$(i\text{-}C_4H_9)_3SiH$	355.0	357.3	0.6	355.8	0.2	348.7	1.8	397.5	12.0	188
$(i\text{-}C_5H_{11})_3SiH$	413.0	419.4	1.5	417.7	1.1	410.5	0.6	459.3	11.2	188
$CH_3(C_2H_5)_2SiH$	200.0	199.7	0.1	201.1	0.5	204.5	2.3	253.4	26.7	188
$CH_3(C_3H_7)_2SiH$	240.0	241.1	0.5	242.4	1.0	245.7	2.4	294.6	22.7	188
$CH_3(C_4H_9)_2SiH$	283.0	282.5	0.2	283.6	0.2	286.9	1.4	335.8	18.7	188
$CH_3(C_5H_{11})_2SiH$	325.0	324.0	0.3	324.9	0.0	328.1	1.0	377.0	16.0	188
$CH_3(C_6H_{13})_2SiH$	366.0	365.4	0.2	366.1	0.0	369.3	0.9	418.2	14.3	188
$CH_3[CH_3(CH_2)_9]_2SiH$	531.0	531.1	0.0	531.1	0.0	534.1	0.6	583.0	9.8	188
$CH_3(i\text{-}C_3H_7)_2SiH$	255.0	253.8	0.5	235.3	7.7	245.7	3.6	294.6	15.5	188
$(C_3H_7)_2(C_2H_5)SiH$	259.0	258.4	0.2	255.3	1.4	266.3	2.8	315.1	21.7	188
$(C_4H_9)_2(C_2H_5)SiH$	301.0	299.8	0.4	296.5	1.5	307.5	2.2	356.3	18.4	188
$(C_5H_{11})_2(C_2H_5)SiH$	340.0	341.3	0.4	337.8	0.7	348.7	2.6	397.5	16.9	188
$(C_6H_{13})_2(C_2H_5)SiH$	381.0	382.7	0.4	379.0	0.5	389.9	2.3	438.7	15.2	188
$(C_8H_{17})_2(C_2H_5)SiH$	468.0	465.5	0.5	461.6	1.4	472.3	0.9	521.1	11.4	188
$(C_{10}H_{21})_2(C_2H_5)SiH$	545.0	548.4	0.6	544.1	0.2	554.7	1.8	603.5	10.7	188
$(i\text{-}C_3H_7)_2(C_2H_5)SiH$	270.0	271.1	0.4	248.2	8.1	266.3	1.4	315.1	16.7	188
$(i\text{-}C_4H_9)_2(C_2H_5)SiH$	315.0	310.6	1.4	308.6	2.0	307.5	2.4	356.3	13.3	188
$(i\text{-}C_5H_{11})_2(C_2H_5)SiH$	358.0	352.0	1.7	350.0	2.2	348.7	2.6	397.5	11.0	188
$(CH_3)_2SiH_2$	94.7	106.0	11.9	103.8	9.6	97.4	2.9	131.8	39.1	45, 66, 141, 181, 182

Table A.1. (Continued)

compound	Exptl	new group contribution		O'Neal and Ring group contribution		new bond contribution		O'Neal and Ring bond contribution		ref
	$-\Delta H^\circ_f$	$-\Delta H^\circ_f$	% dev	$-\Delta H^\circ_f$	% dev	$-\Delta H^\circ_f$	% dev	$-\Delta H_f$	% dev	
$(C_2H_5)_2SiH_2$	182.5	140.6	23.0	129.6	29.0	138.6	24.0	172.9	5.2	66, 141, 142, 143, 181, 182
CH_3SiH_3	29.1	81.6	180.0	33.9	16.5	31.6	8.5	51.2	76.1	45, 66, 141
$C_2H_5SiH_3$	116.9	98.9	15.4	46.3	60.0	52.2	55.4	71.8	38.6	66, 181, 182
$(n\text{-}C_4H_9)SiH_3$	133.8	140.3	4.9	88.0	34.2	93.4	30.2	113.0	15.6	181
$(i\text{-}C_4H_9)SiH_3$	129.6	145.6	12.3	94.1	27.4	93.4	28.0	113.0	12.8	181
$Si(CH_3)_4$	229.0	229.1	0.0	247.3	8.0	229.2	0.1	292.8	27.9	29, 45, 66, 141, 142, 143, 170, 181, 188, 189, 190, 191
$Si(C_2H_5)_4$	297.0	298.3	0.4	298.9	0.6	331.6	4.9	375.0	26.3	66, 86, 141, 142, 143, 181, 182, 184, 188, 189, 190
$Si(C_3H_7)_4$	378.0	381.1	0.8	381.4	0.9	394.0	4.2	457.4	21.0	188, 189, 190
$CH_3Si(C_2H_5)_3$	281.0	281.0	0.0	286.0	1.8	291.0	3.6	354.5	26.1	188, 189, 190
$CH_3Si(C_3H_7)_3$	343.0	343.1	0.0	347.8	1.4	352.8	2.9	416.3	21.4	188, 189, 190
$(CH_3)_2Si(C_2H_5)_2$	263.0	263.7	0.3	273.1	3.8	270.4	2.8	333.9	27.0	188, 189, 190
$(CH_3)_2Si(C_3H_7)_2$	306.0	318.3	4.0	314.3	2.7	311.6	1.8	375.1	22.6	181, 188, 189, 190
$(C_2H_5)_2Si(C_3H_7)_2$	341.0	339.7	0.4	340.1	0.3	352.8	3.5	416.2	22.1	188, 189, 190
$(C_2H_5)_3SiC_3H_7$	319.0	319.0	0.0	319.5	0.2	332.2	4.1	395.6	24.0	188
$C_2H_5Si(C_3H_7)_3$	360.0	360.4	0.1	360.7	0.2	373.4	3.7	436.8	21.3	188
$(C_3H_7)_2Si(C_4H_9)_2$	423.0	422.5	0.1	422.6	0.1	435.2	2.9	498.6	17.9	188
$C_3H_7Si(C_4H_9)_3$	444.0	443.2	0.2	443.3	0.2	455.8	2.7	519.2	16.9	188
$C_2H_5Si(CH_3)_3$	247.4	246.4	0.4	250.2	5.2	249.8	1.0	313.4	26.7	66, 141
$Si[Si(CH_3)_3]_4$	559.3	559.3	*	695.0	24.3	588.4	5.2	762.5	36.3	142
$(OCH_3)_3SiH$	797.5	797.2	0.0	-	-	876.4	9.9	940.4	17.9	66, 146, 182
$(OC_2H_5)_3SiH$	903.4	903.9	0.1	-	-	938.2	3.9	1002.2	10.9	66, 146, 182
$(CH_3)_3SiOC_2H_5$	499.0	490.5	1.7	-	-	487.5	2.3	556.1	11.4	7, 93, 182, 188, 190
$(CH_3)_3SiOC_3H_7$	521.0	511.2	1.9	-	-	508.1	2.5	576.7	10.7	93, 182, 188, 190
$(CH_3)_3SiOCH(CH_3)_2$	524.0	525.2	0.2	-	-	508.1	3.0	576.7	10.1	66, 93, 182, 188, 190
$(CH_3)_3SiO(t\text{-}C_4H_9)$	564.8	564.4	0.1	-	-	528.7	6.4	597.3	5.8	182
$(OC_2H_5)_2Si(CH_3)_2$	775.0	765.5	1.2	-	-	745.8	3.8	819.4	5.7	66, 93, 179, 182, 188, 190
$(OC_2H_5)_2Si(C_3H_7)_2$	852.0	841.5	1.2	-	-	828.2	2.8	901.7	5.8	93, 179, 183, 188, 190
$CH_3Si(OCH_3)_3$	944.0	937.1	0.7	-	-	942.3	0.2	1020.9	8.1	93, 178, 182, 188, 190
$CH_3Si(OC_2H_5)_3$	1045.0	1043.8	0.1	-	-	1004.1	3.9	1082.7	3.6	93, 188, 190
$Si(OCH_3)_4$	1180.0	1188.2	0.7	-	-	1268.0	*	1263.6	7.1	66, 93, 146, 180, 188, 190
$Si(OC_2H_5)_4$	1314.6	1330.4	1.2	-	-	1262.4	4.0	1346.0	2.4	62, 66, 93, 146, 182, 190
$Si(OC_3H_7)_4$	1397.0	1413.3	1.2	-	-	1344.8	3.7	1428.4	2.2	93, 188, 190
$Si(O\text{-}i\text{-}C_3H_7)_4$	1442.8	1469.0	1.8	-	-	1344.8	6.8	1428.4	1.0	146, 182
$Si(OC_4H_9)_4$	1482.0	1496.1	1.0	-	-	1427.2	3.7	1510.8	1.9	188
$(OC_2H_5)_3SiCl$	1176.5	1176.5	*	-	-	1112.5	5.4	1168.4	0.7	62
CH_3SiF_3	1232.7	1232.7	*	-	-	1434.1	2.9	1278.3	3.7	29
$(CH_3)_2SiCl_2$	448.3	448.3	*	-	-	446.0	0.5	464.4	3.6	35, 66, 79, 141, 142,143, 148, 182
$(CH_3)_3SiCl$	353.8	353.8	*	-	-	337.6	4.6	378.6	7.0	7, 8, 10, 35, 66, 141, 142, 182, 191
$(CH_3)_3SiBr$	293.2	293.2	*	-	-	275.8	5.9	322.1	9.9	8, 35, 66, 141, 142, 143, 182
$(CH_3)_3SiI$	206.9	206.9	*	-	-	199.5	3.6	248.9	20.3	141
$(CH_3)_3Si(OH)$	499.5	505.1	1.1	-	-	503.7	0.8	550.1	10.1	8, 35, 141, 142, 143, 182
$(C_2H_5)_2Si(OH)_2$	825.9	829.2	0.4	-	-	819.4	0.8	848.6	2.5	179
CH_3SiHCl_2	402.0	402.0	*	-	-	380.1	5.4	383.9	4.5	35, 66, 79, 142, 143, 182
$CH_3Si(CH_2Cl)Cl_2$	521.7	521.7	*	-	-	460.9	11.6	479.2	8.1	66
$(CH_3)_2SiHCl$	292.6	292.6	*	-	-	271.7	7.1	298.1	1.9	66, 79, 142, 143, 182
CH_3SiCl_3	571.8	550.1	3.8	-	-	554.4	3.0	550.2	3.8	29, 66, 141, 142, 143, 182
$C_2H_5SiCl_3$	512.7	529.4	3.8	-	-	575.0	12.2	570.8	10.2	64, 66, 182
Si_2OF_6	2905.0	2905.0	*	-	-	2815.8	3.1	2845.1	2.1	155
Si_2H_6	-79.9	-79.9	*	-79.9	0.0	-76.3	4.5	-71.5	10.5	55, 66, 77, 141, 191
Si_3H_8	-120.9	-120.9	*	-119.7	1.0	-118.2	2.2	-113.8	5.9	55, 78, 141, 191
Si_2F_6	2366.3	2366.3	*	-	-	2397.4	1.3	2382.6	0.7	6, 141
Si_3F_8	3161.4	3161.4	*	-	-	3180.0	0.6	3158.4	0.1	141
Si_2Cl_6	987.4	987.4	*	-	-	969.4	1.8	926.4	6.2	66
$Si_2(CH_3)_6$	363.1	364.6	0.4	358.2	1.4	319.0	12.1	411.6	13.4	66, 86, 141, 142, 143, 170, 182
$Si_2(C_2H_5)_6$	381.1	468.4	22.9	435.5	14.3	442.6	16.1	534.9	40.4	182, 184
$Si_3(CH_3)_8$	470.4	467.3	0.7	472.1	0.4	408.8	13.1	530.4	12.8	141, 142, 143 189, 191
$Si_4(CH_3)_{10}$	568.4	569.9	0.3	586.0	3.1	499.6	12.3	649.2	14.2	141, 142, 143
$Si_2(OCH_3)_6$	1874.2	1874.2	*	-	-	1745.2	6.9	1867.8	0.3	180, 182

Table A.1. (Continued)

compound	Exptl $-\Delta H^\circ_f$	new group contribution		O'Neal and Ring group contribution		new bond contribution		O'Neal and Ring bond contribution		ref
		$-\Delta H^\circ_f$	% dev	$-\Delta H^\circ_f$	% dev	$-\Delta H^\circ_f$	% dev	$-\Delta H_f$	% dev	
MM	815.4	801.0	1.8	-	-	737.4	9.6	874.4	7.2	7, 35, 67, 86, 141
MDM	1380.7	1386.5	0.4	-	-	1245.6	9.8	1456.0	5.5	141, 142, 143, 182
MD_2M	1934.6	1971.9	1.9	-	-	1753.8	9.3	2037.6	5.3	141, 142, 143, 182
MD_3M	2567.9	2557.3	0.4	-	-	2262.0	11.9	2619.2	2.0	141, 142, 143, 182
M'D'M'	2232.6	2300.3	3.0	-	-	2434.1	9.0	2664.5	19.6	178, 182
$Si_2O(OCH_3)_6$	2267.5	2267.4	0.0	-	-	2163.6	4.6	2330.0	2.8	180, 182
$Si_3O_2(OCH_3)_8$	3380.3	3346.7	1.0	-	-	3147.2	6.9	3397.6	0.5	180, 182
$[Si(OCH_3)_2(CH_3)]_2$	1752.8	1752.8	*	-	-	1269.8	27.6	1382.4	21.1	178, 182
$[Si(OCH_3)_2(C_2H_5)]_2O$	1789.4	1799.8	0.6	-	-	1729.4	3.4	1886.3	5.4	178, 182
$(C_2H_5O)_3Si(CH_2)_3NH_2$	1133.9	1047.1	7.7	-	-	1012.2	10.7	1090.4	3.8	182
$(C_2H_5O)_3Si(CH_2)_2CN$	1075.3	924.7	14.0	-	-	-	-	-	-	182
$Si(C_6H_5)_4$	-333.9	333.9	*	-	-	-333.9	*	-175.7	47.4	14, 169, 182, 183, 184
$O[(CH_3)_2Si(OH)]_2$	1385.8	1380.1	0.4	-	-	1242.4	10.3	1388.9	0.2	67
$(C_6H_5)_2SiCl_2$	208.8	208.8	*	-	-	164.4	21.3	230.2	10.2	35, 143, 148, 182
$(C_6H_5)_2(CH_3)SiH$	-113.0	-114.7	1.5	-	-	-118.3	4.7	-21.9	80.6	188
$(C_6H_5)_2(C_2H_5)SiH$	-94.0	-92.9	1.2	-	-	-97.7	3.9	-1.3	98.6	188
$(CH_3)_3SiOC_6H_5$	385.0	374.3	2.5	-	-	-	-	-	-	188
$(CH_3)_3Si(2\text{-}CH_3OC_6H_4)$	418.0	407.3	2.6	-	-	-	-	-	-	188
$(CH_3)_3Si(3\text{-}CH_3OC_6H_4)$	422.0	407.3	3.5	-	-	-	-	-	-	188
$(CH_3)_3Si(4\text{-}CH_3OC_6H_4)$	418.0	407.3	2.6	-	-	-	-	-	-	188
$(CH_3)_2Si(OC_6H_5)_2$	542.0	533.1	1.6	-	-	-	-	-	-	188
$(CH_3)_2Si(2\text{-}CH_3C_6H_4O)_2$	605.0	594.1	1.8	-	-	-	-	-	-	188
$(CH_3)_2Si(3\text{-}CH_3C_6H_4O)_2$	609.0	598.9	1.7	-	-	-	-	-	-	188
$(CH_3)_2Si(4\text{-}CH_3C_6H_4O)_2$	605.0	598.9	1.0	-	-	-	-	-	-	188
$CH_3Si(OC_6H_5)_3$	698.0	695.1	0.4	-	-	-	-	-	-	188
$CH_3Si(2\text{-}CH_3C_6H_4O)_3$	800.0	786.8	1.7	-	-	-	-	-	-	188
$CH_3Si(3\text{-}CH_3C_6H_4O)_3$	810.0	793.9	2.0	-	-					188
$CH_3Si(4\text{-}CH_3C_6H_4O)_3$	791.0	814.8	2.9	-	-	-	-	-	-	188
$(C_6H_5)Si(C_2H_5O)_3$	904.0	904.0		-	-	881.4	2.5	928.0	2.7	188, 190
$(C_6H_5COOCH_2)Si(OC_2H_5)_3$	1265.0	1265.0	*	-	-	-	-	-	-	93, 188, 190
$(CH_3)_3SiOOC(CH_3)_3$	486.4	486.4		-	-	438.8	9.7	507.3	4.2	145, 182
$Si(OC_6H_5)_4$	1315.0	1333.6	1.4	-	-	-	-	-	-	188
$Si(2\text{-}CH_3C_6H_4O)_4$	989.0	987.8	0.1	-	-	-	-	-	-	188
$Si(3\text{-}CH_3C_6H_4O)_4$	1002.0	997.3	0.5	-	-	-	-	-	-	188
$Si(4\text{-}CH_3C_6H_4O)_4$	976.0	997.3	2.2	-	-	-	-	-	-	188
$Si(CH_3)_3NH(CH_3)$	227.1	-	-	-	-	245.1	7.9	356.4	56.9	8, 35, 141, 142, 143, 182
$(CH_3)_3SiN(CH_3)_2$	247.7	-	-	-	-	243.4	1.7	354.7	43.2	8, 10, 35, 141, 142, 143, 182
$(CH_3)_3SiN(C_2H_5)_2$	329.5	-	-	-	-	284.6	13.6	395.9	20.2	32, 142, 143, 182
$(C_2H_5)_3SiN(C_2H_5)_2$	331.7	-	-	-	-	346.4	4.4	457.7	38.0	95, 182
$[(CH_3)_3Si]_2NH$	476.6	-	-	-	-	460.9	3.3	683.5	43.4	8, 35, 141, 142, 143, 182
$[(CH_3)_3Si]_2N(CH_3)$	448.3	-	-	-	-	459.2	2.4	681.8	52.1	8, 35, 141, 142, 143, 182
$[(CH_3)_3Si]_3N$	670.3	-	-	-	-	675.0	0.7	1008.9	50.5	8, 35, 141, 142
$(CH_3)_3SiSC_4H_9$	340.9	-	-	-	-	340.9	*	-	-	35, 141, 142
SiH_4	-34.3	-	-	-	-	-34.3	*	29.2	14.9	29, 66, 141, 191
SiF_3H	1225.9	-	-	-	-	1202.5	1.9	1197.8	2.3	29, 51, 141
SiF_2H_2	804.2	-	-	-	-	790.2	1.7	788.8	1.9	29, 51, 141
$SiFH_3$	415.9	-	-	-	-	378.0	9.1	379.8	8.7	29, 51, 141
SiF_4	1614.9					1614.8		1606.8	0.5	29, 66, 141, 191
$SiCl_4$	662.8	-	-	-	-	662.8	*	636.0	4.0	29, 66, 141, 191
$SiCl_3H$	499.2	-	-	-	-	488.5	2.1	469.7	5.9	29, 53, 66, 141, 191
$SiCl_2H_2$	315.1	-	-	-	-	314.2	0.3	303.4	3.7	29, 53, 141
$SiClH_3$	135.6	-	-	-	-	140.0	3.2	137.1	1.1	29, 53, 141
$SiBr_4$	415.5	-	-	-	-	415.6	*	410.0	1.3	29, 66, 141, 191
$SiBr_3H$	303.3	-	-	-	-	303.1	0.1	300.2	1.0	52, 141, 142, 191
$SiBr_2H_2$	180.7	-	-	-	-	190.6	5.5	190.4	5.4	29, 52, 142
$SiBrH_3$	64.0	-	-	-	-	78.2	22.1	80.6	25.9	29, 52, 142
SiI_4	110.5	-	-	-	-	110.5	*	117.2	6.1	29, 141
$SiFCl_3$	841.0	-	-	-	-	900.8	7.1	878.7	4.5	29, 141
SiF_3Cl	1318.9	-	-	-	-	1376.8	4.5	1364.1	3.5	29, 141
	138.2	138.2	*	-	-	138.2	*	-	-	35, 141, 142, 143
	181.6	181.6	*	-	-	181.6	*	-	-	35, 141, 142, 143
av % dev			1.9		5.4		5.7		17.3	
% bias			-0.2		-1.5		-2.0		12.4	

[a] All $\Delta H^\circ_{f,298}$ are in kilojoules per mole, and deviations are absolute. Accepted references are underlined. Molecule abbreviations: M = $(CH_3)_3SiO_{0.5}$, D = $(CH_3)_2SiO$, M′ = $(CH_3)(OCH_3)_2SiO_{0.5}$, D′ = $(CH_3)(OCH_3)SiO$. [b] **Asterisks designate compounds from which a group contribution value has been directly derived.** The percentage deviation would then, of course, be zero.

Table A.2. Predictions of the Standard Ideal Gas Enthalpy of Formation at 298.15 K for Boron and Aluminum Compounds[a,b]

compound	exptl $-\Delta H^\circ_f$	new group contribution $-\Delta H^\circ_f$	new group contribution % dev	Benson group contribution $-\Delta H^\circ_f$	Benson group contribution % dev	ref
$B(CH_3)_3$	122.8	122.8	0.0	122.7	0.1	35, 57, 75, 191, 142, 143, 160, 182
$B(C_2H_5)_3$	148.8	152.3	2.4	150.6	1.2	35, 57, 75, 191, 142, 143, 160, 182
$B(C_3H_7)_3$	236.7	214.5	9.4	212.7	10.1	35, 57, 75, 142, 143, 182
$B(i\text{-}C_3H_7)_3$	252.1	213.9	15.2	225.5	10.6	35, 57, 75, 142, 143, 182
$B(C_4H_9)_3$	290.6	276.7	4.8	274.8	5.4	35, 57, 75, 142, 143, 160, 182
$B(i\text{-}C_4H_9)_3$	278.3	292.7	5.2	291.0	4.6	35, 75, 142, 143, 160, 182
$B(s\text{-}C_4H_9)_3$	245.0	267.3	9.1	267.5	9.2	35, 75, 142, 143, 160, 182
$B(C_5H_{11})_3$	378.5	338.7	10.5	337.0	11.0	75
$B(s\text{-}C_5H_{11})_3$	381.8	354.8	7.1	363.1	4.9	35, 75, 142, 143, 182
$B(C_6H_{13})_3$	397.4	400.8	0.9	399.1	0.4	35, 57, 75, 142, 143, 160, 182
$B(C_7H_{15})_3$	456.8	463.0	1.4	461.2	1.0	35, 57, 75, 142, 143, 160, 182
$B(C_8H_{17})_3$	515.2	524.7	1.8	523.3	1.6	35, 57, 75, 142, 143, 160, 182
$B(s\text{-}C_8H_{17})_3$	518.8	515.7	0.6	526.0	1.4	35, 75, 142, 182
$B(OCH_3)_3$	900.1	918.7	2.1	896.5	0.4	35, 56, 75, 191, 142, 182
$B(OC_2H_5)_3$	1001.7	1025.4	2.4	1003.2	0.1	35, 57, 75, 191, 142, 161, 182
$B(OC_3H_7)_3$	1076.4	1087.5	1.0	1065.3	1.0	35, 57, 75, 142, 182
$B(OC_4H_9)_3$	1147.0	1149.6	0.2	1127.5	1.7	35, 56, 75, 142, 182
$HB(OCH_3)_2$	580.7	576.5	0.7	582.5	0.3	34, 35, 57, 75, 191, 142, 182
$HB(i\text{-}OC_3H_7)_2$	732.2	715.3	2.3	721.2	1.5	12, 57, 75
$B_2(OCH_3)_4$	1126.1	1136.7	0.9	-	-	142
$B(SCH_3)_3$	156.2	204.4	30.9	206.0	31.9	35, 57, 59, 75, 142, 182
$B(SC_2H_5)_3$	280.8	275.4	1.9	276.9	1.4	35, 57, 75, 142, 182
$B(SC_3H_7)_3$	333.4	337.5	1.2	339.1	1.4	35, 57, 59, 75, 142, 182
$B(SC_4H_9)_3$	394.1	399.6	1.4	401.2	1.8	35, 57, 59, 75, 142, 182
$B(SC_5H_{11})_3$	462.9	461.7	0.3	463.3	0.1	35, 57, 59, 75, 142, 182
$BNOC_9H_{22}$	553.2	553.2	*	-	-	65, 142, 182
$B(N(CH_3)_2)_3$	245.4	254.4	3.7	276.2	12.6	35, 57, 142, 182
$(CH_3)_2BNH(CH_3)$	340.6	383.8	12.7	-	-	143
$(C_2H_5)_2BNH(C_2H_5)$	550.6	437.8	20.5	-	-	143
$(C_3H_7)_2BC_3H_6N(CH_3)_2$	251.0	178.8	28.8	177.1	29.4	182
$(C_3H_7)_2BN(C_3H_7)_2$	372.4	368.7	1.0	-	-	182
$(C_4H_9)_2BN(C_4H_9)_2$	447.7	451.6	0.9	-	-	182
$(N(CH_3)_2)_2BCl$	334.8	334.8	*	351.8	5.1	35, 57, 75, 142, 182
$(N(CH_3)_2)BCl_2$	401.3	401.3	*	410.2	2.2	35, 57, 75, 142, 182
$H_2B(OH)$	290.4	290.4	*			75, 144
$HB(OH)_2$	640.5	661.8	3.3	883.2	37.9	75, 144
$B_2(OH)_4$	1317.8	1307.2	0.8	-	-	75
$(C_4H_9)_2B(OH)$	552.8	552.8	*	546.4	1.2	75, 142, 143, 160, 182
F_2BOH	1090.6	1090.6	*	-	-	75, 191
$FB(OH)_2$	1042.7	1042.7	*	-	-	75, 191
CH_3BF_2	832.6	848.4	1.9	828.3	5.3	160
$F_2BC_2H_5$	874.5	874.8	0.0	837.6	0.6	160
$F_2B(i\text{-}C_3H_7)$	887.0	895.5	1.0	865.9	2.4	160
B_2F_4	1431.8	1431.8	*	-	-	29, 57, 75, 76, 191
B_2Cl_4	489.1	489.1	*	-	-	29, 57, 191
$O(BF_2)_2$	1898.1	1898.1	*	-	-	29
$(CH_3O)_2BCl$	746.3	750.5	0.6	748.2	0.3	35, 57, 75, 142, 182, 191
$(OC_2H_5)_2BCl$	819.8	818.7	0.1	819.3	0.1	35, 57, 75, 142, 161, 182, 191
$(OC_2H_5)BCl_2$	623.3	623.3	*	624.5	0.2	35, 57, 75, 142, 161, 182, 191
$(C_4H_9)_2BCl$	368.8	368.8	*	363.9	1.3	35, 57, 75, 142, 161, 182, 191
$(C_4H_9)_2BBr$	305.2	305.2	*	297.8	2.4	35, 57, 75, 142, 143, 182, 191
$(C_4H_9)_2BI$	229.4	229.4	*	222.5	3.0	35, 57, 75, 142, 160
$(t\text{-}C_4H_9O_2)_3B$	1016.7	1087.2	6.9	-	-	182
$s\text{-}C_4H_9O_2B(OC_4H_9)_2$	1104.6	1063.5	3.7	-	-	182
$(s\text{-}C_4H_9O_2)_2BOC_4H_9$	1062.7	977.4	8.0	-	-	182
$B(C_6H_5)_3$	-129.9	-129.9	*	-	-	35, 57, 58, 142, 182
$B(OC_6H_5)_3$	591.9	593.1	0.2	-	-	56, 182
$B(SC_6H_5)_3$	-191.9	-191.9	*	-211.2	10.1	35, 56, 59, 75
$B(m\text{-}CH_3C_6H_4O)_3$	690.2	703.1	1.9	-	-	182, 199
$B(p\text{-}CH_3C_6H_4O)_3$	680.5	703.4	3.4	-	-	182, 199
$C_6H_5BCl_2$	266.0	249.5	6.2	-	-	35, 57, 58, 75, 142
$(C_6H_5)_2BCl$	93.5	93.5	*	-	-	35, 57, 58, 142, 182
$(o\text{-}CH_3C_6H_4)BCl_2$	253.8	280.0	10.3	-	-	60, 182
$(p\text{-}CH_3C_6H_4)BCl_2$	294.1	282.4	4.0	-	-	60, 182
$B(m\text{-}ClC_6H_4O)_3$	706.2	688.6	2.5	-	-	182, 199
$B(p\text{-}ClC_6H_4O)_3$	711.3	688.6	3.2	-	-	182, 199
$C_6H_5BBr_2$	129.3	129.3	*	-	-	35, 57, 58, 75, 142, 182
$(C_6H_5)_2BBr$	9.4	9.4	*	-	-	35, 57, 58, 142, 182
$(C_6H_5)B(OH)_2$	635.0	635.0	*	-	-	75
$[(C_6H_5)_2B]_2O$	266.0	266.0	*	-	-	75
$Al(CH_3)_3$	81.3	81.3	0.0	88.1	8.4	35, 120, 142, 143 160, 182, 191
$Al(C_2H_5)_3$	163.6	166.4	1.7	156.8	4.2	35, 142, 143, 153, 160, 182
$Al(C_3H_7)_3$	239.1	228.5	4.4	218.9	8.4	142, 143, 156, 182
$Al(i\text{-}C_4H_9)_3$	255.2	263.4	3.2	253.8	0.5	154, 182

Table A.2. (Continued)

compound	exptl $-\Delta H^\circ_f$	new group contribution $-\Delta H^\circ_f$	new group contribution % dev	Benson group contribution $-\Delta H^\circ_f$	Benson group contribution % dev	ref
$HAl(C_2H_5)_2$	146.5	150.1	2.5	-	-	142, 143, 153
$HAl(i\text{-}C_4H_9)_2$	247.1	243.7	1.4	-	-	142, 153
$(C_2H_5)_2AlCl$	415.1	406.3	2.1	-	-	152
$(i\text{-}C_4H_9)_2AlCl$	491.0	499.9	1.8	-	-	154
Al_2Cl_4	811.7	811.7	*	-	-	1
			Boron Compounds			
av % dev			4.8		5.3	
% bias			-0.5		0.2	
			Aluminum Compounds			
av % dev			2.1		6.2	
% bias			0.2		-1.2	

[a] All $\Delta H^\circ_{f,298}$ are in kilojoules per mole, and deviations are absolute. Accepted references are underlined. [b] Asterisks indicate compounds from which a group contribution value has been directly derived. The percentage deviation would then, of course, be zero.

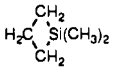
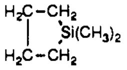
Table A.3. Predictions of the Enthalpy of Vaporization at 298.15 K for Silicon Compounds[a,b]

compound	exptl $\Delta H_{v,298}$	group method $\Delta H_{v,298}$	group method % dev	acentric factor method ω	acentric factor method $\Delta H_{v,298}$	acentric factor method % dev	ref
$(CH_3)_3SiH$	24.4	28.1	15.2	-	-	-	141, 181
$(C_2H_5)_3SiH$	36.4	33.8	7.2	-	-	-	141, 142, 188
$(C_3H_7)_3SiH$	39.1	38.1	2.6	-	-	-	188
$(C_4H_9)_3SiH$	42.9	42.4	1.2	-	-	-	188
$(C_5H_{11})_3SiH$	48.1	46.7	3.0	-	-	-	188
$(C_6H_{13})_3SiH$	51.0	51.0	0.0	-	-	-	188
$(C_7H_{15})_3SiH$	57.4	55.2	3.8	-	-	-	188
$(C_8H_{17})_3SiH$	59.8	59.5	0.5	-	-	-	188
$(C_9H_{19})_3SiH$	61.8	63.8	3.3	-	-	-	188
$(C_{10}H_{21})_3SiH$	65.3	68.1	4.3	-	-	-	188
$(i\text{-}C_4H_9)_3SiH$	40.0	40.7	1.7	-	-	-	188
$(i\text{-}C_5H_{11})_3SiH$	43.8	45.0	2.7	-	-	-	188
$CH_3(C_2H_5)_2SiH$	34.6	31.9	7.8	-	-	-	188
$CH_3(C_3H_7)_2SiH$	35.9	34.8	3.2	-	-	-	188
$CH_3(i\text{-}C_3H_7)_2SiH$	32.4	35.5	9.7	-	-	-	188
$CH_3(C_4H_9)_2SiH$	36.2	37.6	3.9	-	-	-	188
$CH_3(C_5H_{11})_2SiH$	40.3	40.5	0.4	-	-	-	188
$CH_3(C_6H_{13})_2SiH$	42.6	43.3	1.7	-	-	-	188
$CH_3[CH_3(CH_2)_9]_2SiH$	57.4	54.8	4.6	-	-	-	188
$(C_3H_7)_2(C_2H_5)SiH$	37.9	36.7	3.3	-	-	-	188
$(C_4H_9)_2(C_2H_5)SiH$	39.9	39.5	1.0	-	-	-	188
$(C_5H_{11})_2(C_2H_5)SiH$	41.2	42.4	2.8	-	-	-	188
$(C_6H_{13})_2(C_2H_5)SiH$	44.8	45.2	1.0	-	-	-	188
$(C_8H_{17})_2(C_2H_5)SiH$	47.3	50.9	7.7	-	-	-	188
$(C_{10}H_{21})_2(C_2H_5)SiH$	58.7	56.7	3.5	-	-	-	188
$(i\text{-}C_3H_7)_2(C_2H_5)SiH$	38.1	37.4	1.8	-	-	-	188
$(i\text{-}C_4H_9)_2(C_2H_5)SiH$	39.8	38.4	3.5	-	-	-	188
$(i\text{-}C_5H_{11})_2(C_2H_5)SiH$	42.6	41.3	3.2	-	-	-	188
$(CH_3)_2SiH_2$	21.3	23.0	7.7	-	-	-	141
$(C_2H_5)_2SiH_2$	30.0	26.7	10.9	-	-	-	141, 142, 181
CH_3SiH_3	18.4	24.4	32.6	-	-	-	141
$C_4H_9SiH_3$	28.5	29.1	2.2	-	-	-	181
$(i\text{-}C_4H_9)SiH_3$	29.2	28.6	2.1	-	-	-	181
$Si(CH_3)_4$	26.1	33.5	28.4	0.239	24.5	6.3	39, *61*, 141, 142, 170, 174, 181, 188, 190, 191
$Si(C_2H_5)_4$	39.8	41.0	3.0	0.463	47.4	19.0	39, 141, 142, *174*, 188, 190
$Si(C_3H_7)_4$	42.2	46.7	10.7	-	-	-	188, 190
$CH_3Si(C_2H_5)_3$	40.5	39.1	3.4	0.411	41.5	2.5	*174*, 188, 190
$C_3H_7Si(C_2H_5)_3$	46.5	42.4	8.7	0.518	51.7	11.4	*174*
$C_4H_9Si(C_2H_5)_3$	49.0	43.9	10.5	0.522	55.3	12.8	*174*
$C_5H_{11}Si(C_2H_5)_3$	52.0	45.3	12.9	0.609	59.9	15.2	*174*
$C_6H_{13}Si(C_2H_5)_3$	53.3	48.2	9.6	0.674	65.9	23.6	*174*
$CH_3Si(C_3H_7)_3$	42.6	43.4	1.9	-	-	-	188, 190
$(CH_3)_2Si(C_2H_5)_2$	38.9	37.2	4.3	-	-	-	188, 190
$(CH_3)_2Si(C_3H_7)_2$	40.2	40.1	0.3	-	-	-	188, 190
$(C_2H_5)_2Si(C_3H_7)_2$	41.5	43.9	5.7	-	-	-	188, 190
$(C_4H_9)_2Si(CH_7)_2$	44.0	49.6	12.7	-	-	-	188
$C_2H_5Si(CH_3)_3$	30.1	35.3	17.4	-	-	-	141, 174
$C_3H_7Si(CH_3)_3$	32.8	36.8	12.1	0.351	35.4	7.8	*174*
$C_4H_9Si(CH_3)_3$	39.0	38.2	2.1	0.410	40.3	3.2	*174*
$C_5H_{11}Si(CH_3)_3$	41.5	39.6	4.5	0.443	43.9	5.7	*174*
$C_6H_{13}Si(CH_3)_3$	44.6	41.4	7.9	0.513	49.6	11.2	*174*
$C_7H_{15}Si(CH_3)_3$	48.0	42.5	11.5	0.549	53.3	11.0	*174*
$C_8H_{17}Si(CH_3)_3$	53.9	43.9	18.5	0.631	59.3	10.1	*174*
$C_2H_5Si(C_3H_7)_3$	41.0	45.3	10.5	-	-	-	188
$C_3H_7Si(C_2H_5)_3$	40.0	42.4	6.1	-	-	-	188

Table A.3. (Continued)

		group method		acentric factor method			
compound	exptl $\Delta H_{v,298}$	$\Delta H_{v,298}$	% dev	ω	$\Delta H_{v,298}$	% dev	ref
$C_3H_7Si(C_4H_9)_3$	45.0	51.0	13.4	-	-	-	188
$(CH_3)_3Si(OH)$	45.6	45.6	*	-	-	-	35, 141, 142
$Si(OCH_3)_4$	41.4	38.5	7.2	-	-	-	93, 188, 190
$Si(OC_2H_5)_4$	48.5	45.3	6.6	0.628	54.2	11.7	93, *174*, 190
$Si(OC_3H_7)_4$	49.8	51.1	2.5	-	-	-	93, 188, 190
$Si(OC_4H_9)_4$	52.0	56.8	9.2	-	-	-	188
$(CH_3O)_3SiCH_3$	34.3	37.1	8.2	-	-	-	93, 188, 190
$(C_2H_5O)_3SiCH_3$	45.1	42.3	6.3	0.651	50.8	12.6	93, *174*, 188, 190
$(C_2H_5O)_2Si(CH_3)_2$	43.1	40.3	6.4	0.519	42.9	0.5	93, *174*, 188, 190
$(C_2H_5O)_2Si(C_3H_7)_2$	46.5	47.0	1.2	-	-	-	188, 190
$(CH_3)_3SiOC_2H_5$	38.4	36.1	6.0	-	-	-	93, 174, 188, 190
$(CH_3)_3SiOC_3H_7$	34.3	37.5	9.4	-	-	-	93, 188
$(CH_3)_3Si(O\text{-}i\text{-}C_3H_7)$	31.8	31.8	*	-	-	-	93, 188, 190
$Si_2(CH_3)_6$	37.4	37.8	1.0	-	-	-	141, 142
$Si_3(CH_3)_8$	46.0	45.2	1.7	-	-	-	141, 142
$Si_4(CH_3)_{10}$	52.3	52.7	0.7	-	-	-	141, 142, 174
$Si(Si[CH_3]_3)_4$	53.1	53.1	*	-	-	-	141, 142
MM	37.3	36.9	1.2	0.419	37.7	1.1	35, *61*, 74, 141, 142, 150, 175, 177, 191
MDM	39.7	41.9	5.6	0.513	46.2	16.4	*61*, 141, 142, 174
MD_2M	48.1	47.0	2.3	0.645	55.9	16.2	*61*, 141, 142, 174
MD_3M	53.1	52.0	2.0	0.741	62.7	18.0	*61*, 141, 142, 174
M'M'	49.4	51.2	3.6	0.649	52.5	6.3	*174*
M'DM'	56.3	56.2	0.1	0.759	60.3	7.1	*174*
M“M”	42.7	46.0	7.6	0.363	41.6	2.5	*164*, *174*
M“DM”	50.2	51.0	1.6	0.506	51.6	2.8	*174*
M“D_2M”	55.4	56.1	1.2	0.654	61.6	11.2	*174*
$[Cl_3Si]_2O$	45.0	49.5	10.0	0.354	54.1	20.2	*174*, *200*
$[Si(C_2H_5)_2Cl]_2O$	59.0	53.5	9.3	0.577	62.4	5.8	*164*
Si_2H_6	19.2	18.7	2.4	-	-	-	141, 200
Si_3H_8	28.0	28.9	3.4	-	-	-	141, 190, 191
Si_4H_{10}	39.6	39.1	1.2	-	-	-	174
Si_2Cl_6	46.9	46.9	*	-	-	-	174
Si_2F_6	27.2	27.2	*	-	-	-	141
Si_3F_8	36.8	36.8	*	-	-	-	141
$C_2H_5SiF_3$	22.7	22.4	1.3	0.392	22.3	1.9	*15*, *48*, *174*
$C_3H_7SiF_3$	26.8	27.4	2.2	0.380	26.0	2.8	*16*
$i\text{-}C_3H_7SiF_3$	25.0	24.2	3.1	0.329	24.0	4.2	*20*
$C_4H_9SiF_3$	31.9	32.4	1.5	0.398	30.1	5.6	*19*
$(CH_3)_2SiF_2$	24.9	26.2	5.2	-	-	-	21
$(C_2H_5)_2SiF_2$	32.1	30.0	6.6	0.349	30.6	4.5	*48*, *174*
$(CH_3)_3SiF$	28.0	28.0	*	-	-	-	21
CH_3SiCl_3	31.0	34.0	9.5	-	-	-	18, 90, 141, 142, 174
$C_2H_5SiCl_3$	37.7	35.9	4.9	0.300	36.8	2.4	*15*, *90*, *174*
$C_3H_7SiCl_3$	41.6	40.8	1.9	0.351	38.8	6.8	*16*
$i\text{-}C_3H_7SiCl_3$	38.0	37.7	0.9	-	-	-	20, 174
$(OC_2H_5)SiCl_3$	36.9	40.7	10.3	0.421	40.5	9.7	*174*
$(CH_3)HSiCl_2$	28.0	28.6	2.2	-	-	-	17, 35, 90, 142, 173, 174
$(C_2H_5)HSiCl_2$	31.3	30.5	2.5	-	-	-	90
$(CH_3)_2SiCl_2$	34.3	36.8	7.4	-	-	-	21, 35, 90, 141, 142, 174
$(C_2H_5)_2SiCl_2$	43.7	40.6	7.1	0.325	41.1	5.9	*90*, *174*
$(OC_2H_5)(CH_3)SiCl_2$	36.6	36.6	*	0.390	38.8	6.0	*174*
$(CH_3)_2HSiCl$	28.5	28.5	*	-	-	-	142
$(CH_3)_3SiCl$	30.1	32.3	7.2	-	-	-	21, 35, 90, 141, 142, 174, 191
$(C_2H_5)_3SiCl$	42.2	37.9	10.1	0.405	44.6	5.7	*174*
CH_3SiCl_2F	28.4	29.1	2.3	-	-	-	18
$C_2H_5SiCl_2F$	31.1	31.0	0.5	-	-	-	15
$i\text{-}C_3H_7SiCl_2F$	34.9	32.8	6.1	-	-	-	20
$C_4H_9SiCl_2F$	39.3	40.9	4.1	0.406	40.2	2.3	*19*
$C_2H_5SiClF_2$	27.4	27.7	0.9	-	-	-	15
$i\text{-}C_3H_7SiClF_2$	31.0	29.5	4.9	0.313	28.3	8.7	*20*
$C_4H_9SiClF_2$	36.1	37.6	4.2	0.399	35.2	2.6	*19*
$CH_3HSiClF$	29.3	29.3	*	-	-	-	17
$(CH_3)_2SiClF$	28.4	28.4	*	-	-	-	21
$(CH_3)_3SiBr$	32.6	32.6	*	-	-	-	35, 141, 142
CH_3SiBrH_2	28.5	28.5	*	-	-	-	46
$(C_6H_5)_2(CH_3)SiH$	64.6	60.4	6.6	0.536	69.6	7.8	*174*, *188*
$(C_6H_5)_2(C_2H_5)SiH$	66.1	62.2	5.8	-	-	-	188
$(C_6H_5)(CH_3)_2SiH$	44.9	44.2	1.5	0.373	46.3	3.0	*174*
$(C_6H_5)(CH_3)_2SiOC_2H_5$	49.9	55.1	10.4	0.321	46.2	7.4	*174*
$(C_6H_5)(OC_2H_5)_2SiCH_3$	59.2	62.2	5.8	0.717	67.1	13.3	*174*
$C_6H_5Si(C_2H_5O)_3$	58.3	67.0	15.0	0.835	74.2	27.3	*174*, *188*, 190
$C_6H_5SiF_3$	36.0	36.6	1.8	0.385	37.9	5.2	*48*, *174*
$(C_6H_5)(CH_3)_2SiCl$	50.1	48.4	3.4	0.398	53.1	6.0	*174*
$(C_6H_5)(CH_3)SiCl_2$	50.5	53.0	4.9	0.406	55.2	9.4	*174*
$(C_6H_5)_2SiCl_2$	69.5	69.1	0.6	0.536	74.3	6.9	35, *90*, 141, *174*
$(C_2H_3)_4Si$	42.7	42.6	0.3	-	-	-	188, 190

Table A.3. (Continued)

		group method		acentric factor method			
compound	exptl $\Delta H_{v,298}$	$\Delta H_{v,298}$	% dev	ω	$\Delta H_{v,298}$	% dev	ref
$(CH_3)_3SiC_2H_3$	33.1	35.7	7.9	-	-	-	188, 190
$(C_2H_5O)_3SiC_2H_3$	50.2	44.5	11.3	0.731	56.1	11.8	*90*, 93, 188, 190
$(C_3H_7O)_3SiC_2H_3$	52.3	48.8	6.7	-	-	-	93, 188, 190
$(C_2H_3)(C_2H_5)SiCl_2$	39.6	38.1	3.9	0.366	41.9	5.9	*90*
$(H_2C{=}CHCH_2)(C_2H_5)SiCl_2$	42.5	43.2	1.6	0.428	46.9	10.3	*174*
$(H_2C{=}CHCH_2)_2SiCl_2$	45.8	45.7	0.2	0.467	50.4	9.9	*174*
$(C_2H_3)SiCl_3$	34.0	36.2	6.6				90
$CH_2{=}CHCH_2SiCl_3$	39.8	38.4	3.5	0.367	40.9	2.7	*90*, *174*
$(CH_3)_3SiN(CH_3)H$	36.0	36.0	0.0	-	-	-	35, 141, 142
$(CH_3)N(SiH_3)_2$	27.7	27.9	0.9	-	-	-	174
$(C_2H_5)N(SiH_3)_2$	29.5	29.3	0.7	-	-	-	174
$(CH_3)_3SiN(CH_3)_2$	31.8	32.6	2.6	-	-	-	35, 141, 142
$(C_2H_5)_3SiN(C_2H_5)_2$	41.8	41.0	1.9	-	-	-	94
$(CH_3)N[Si(CH_3)_3]_2$	38.9	38.9	0.0	-	-	-	35, 141, 142
$(CH_3)_2NSi(CH_3)H_2$	28.2	28.2	0.0	-	-	-	46
$HN[Si(CH_3)_3]_2$	41.4	41.4	*	0.527	43.6	5.0	35, *43*, *74*, 141, 142
$[(C_2H_5)_2N]_3SiH$	58.6	58.6	*	-	-	-	94
$N[Si(CH_3)_3]_3$	54.4	54.4	*	-	-	-	35
	34.7	34.7	*	-	-	-	35, 141, 142, 143
	37.7	37.7	*	-	-	-	35, 141, 142, 143
av % dev			5.3			8.3	
% bias			0.8			6.1	

[a] All $\Delta H_{v,298}$ are in kilojoules per mole, and deviations are absolute. Accepted references are underlined. References from which vapor pressure data were used to determine the acentric factor are italic. Molecule abbreviations: M = $(CH_3)_3SiO_{0.5}$, D = $(CH_3)_2SiO$, M′ = $(CH_3)_2(OC_2H_5)SiO_{0.5}$, M″ = $(CH_3)_2ClSiO_{0.5}$. [b] Asterisks designate compounds from which a group contribution value has been directly derived. The percentage deviation is zero.

Table A.4. Predictions of the Enthalpy of Vaporization at 298.15 K for Boron and Aluminum Compounds[a,b]

		group method		
	exptl $\Delta H_{v,298}$	$\Delta H_{v,298}$	% dev	ref
$B(CH_3)_3$	20.2	20.2	0.0	9, 31, 35, 39, 75, 142, 143, 160, 191
$B(C_2H_5)_3$	36.8	29.6	19.6	31, 35, 39, 75, 107, 142, 143, 160, 191
$B(C_3H_7)_3$	41.8	44.5	6.5	9, 35, 39, 75, 142, 143
$B(i\text{-}C_3H_7)_3$	41.8	41.9	0.2	9, 31, 35, 39, 75, 142, 143
$B(C_4H_9)_3$	61.9	59.5	3.9	35, 39, 75, 142, 143, 160
$B(i\text{-}C_4H_9)_3$	59.8	55.6	7.1	35, 39, 75, 142, 143
$B(s\text{-}C_4H_9)_3$	60.6	56.8	6.2	35, 39, 75, 142, 143
$B(C_5H_{11})_3$	74.1	74.4	0.4	75
$BC_{15}H_{33}$	71.9	70.5	1.9	35, 142
$B(C_6H_{13})_3$	88.7	89.3	0.7	35, 75, 142, 143
$B(C_7H_{15})_3$	102.0	104.3	2.2	35, 75, 142, 143
$B(C_8H_{17})_3$	115.5	119.2	3.2	35, 75, 142, 143
$B(s\text{-}C_8H_{17})_3$	112.9	116.6	3.3	35, 75, 142, 143
$(CH_3)_2BOCH_3$	52.3	54.6	4.3	33
$(CH_3O)_2BC_2H_4B(OCH_3)_2$	54.3	53.7	1.0	185
$(CH_3)_2BC_2H_4B(CH_3)_2$	35.4	35.4	0.0	185
$CH_3B(OH)_2$	36.7	37.8	3.1	25
$(C_4H_9)_2BOH$	62.7	60.4	3.6	75, 142, 143, 185
$B_2(CH_3)_4$	31.4	31.4	*	174
$B_2(CH_3O)_4$	44.7	44.5	0.4	22, 142, 196
$B_2(C_2H_5O)_4$	62.7	62.9	0.3	22
$B(SCH_3)_3$	54.0	56.1	3.8	35, 75, 142
$B(SC_2H_5)_3$	61.5	63.2	2.8	35, 75, 142
$B(SC_3H_7)_3$	87.0	78.1	10.2	35, 75, 142
$B(SC_4H_9)_3$	95.8	93.1	2.8	35, 75, 142
$B(SC_5H_{11})_3$	104.6	108.0	3.3	75, 142
$(C_4H_9)_2BCl$	50.2	50.2	*	35, 75, 142, 143, 160
$(CH_3O)_2BCl$	34.3	32.0	6.7	35, 75, 142, 191, 198
$(C_2H_5O)_2BCl$	38.9	41.2	5.9	75, 142, 191, 198
CH_3OBCl_2	31.8	31.2	2.0	191, 198
$C_2H_5OBCl_2$	35.1	35.8	1.9	35, 75, 142, 198
$Cl_2BC_2H_4BCl_2$	42.2	42.7	1.1	185
B_2Cl_4	31.0	31.0	*	75, 186, 191
$(C_4H_9)_2BBr$	52.3	59.1	13.1	35, 75, 142, 143, 160
$(C_4H_9)_2BI$	54.4	54.4	*	35, 75, 142, 143
$(C_4H_9)B(OCH_3)N(C_2H_5)_2$	58.2	58.2	*	142
$B[N(CH_3)_2]_3$	46.9	46.9	*	27, 35, 75, 142, 197
$B_2[N(CH_3)_2]_4$	54.6	54.6	*	23
$(CH_3)_2NB(CH_3)_2$	31.9	31.9	*	26
$(C_2H_5)_2BNH(C_2H_5)$	60.7	60.7	*	143
$[(CH_3)_2N]_2BH$	38.7	38.7	*	27
$[(CH_3)_2N]_2BF$	38.8	38.8	*	26
$(CH_3)_2N]BCl_2$	37.3	38.1	2.2	35, 75, 142, 197
$(CH_3CH_2)_2NBCl_2$	41.8	40.8	2.4	138
$[(CH_3)_2N]_2BCl$	41.8	41.8	*	35, 75, 142, 197
$C_6H_5BCl_2$	33.9	33.0	2.7	35, 60, 75, 142, 143
$(C_6H_5)_2BCl$	41.4	41.8	1.1	35, 142, 143
$C_6H_5BBr_2$	43.9	43.9	*	35, 75, 142, 143
$(C_6H_5)_2BBr$	60.3	51.2	15.0	35, 142, 143
$(CH_3)_2BC_3H_5$	31.5	30.5	3.3	140
$B(C_2H_3)_3$	33.1	33.4	1.0	140
$(CH_3)B(C_2H_3)_2$	29.3	28.7	2.0	140
$Al(CH_3)_3$	63.2	63.2	0.0	9, 35, 39, 49, 80, 142, 143, 160, 204
$Al(C_2H_5)_3$	73.2	73.1	0.2	35, 39, 142, 143, 204
$Al(C_3H_7)_3$	88.2	88.3	0.1	142, 143, 204
$(CH_3)_2AlCl$	23.2	23.2	*	49
$HAl(C_2H_5)_2$	57.7	57.7	*	35, 142, 143
$HAl(i\text{-}C_4H_9)_2$	42.3	69.4	64.0	35, 142, 143
$(C_2H_5)_2AlOC_2H_5$	48.6	48.6	0.0	142, 143
$(C_2H_5)_2AlOC_3H_7$	53.5	53.5	0.0	142, 143
av % dev			3.4	
% bias			-0.7	

[a] All $\Delta H_{v,298}$ are in kilojoules per mole, and deviations are absolute. Accepted references are underlined. [b] Asterisks designate compounds from which a group contribution value has been directly derived. The percentage deviation would then, of course, be zero.

Table A.5. Revised Harrison–Seaton Method for Prediction of the Ideal Gas Heat Capacity for Organometallic Compounds[a]

	300 K		400 K		500 K		600 K		800 K		1000 K		1500 K		
compound	$C°_p$ (exptl)	% dev	$C°_p$ (exptl)	% dev	$C°_p$ (exptl)	% dev	$C°_p$ (exptl)	% dev	$C°_p$ (exptl)	% dev	$C°_p$ (exptl)	% dev	$C°_p$ (exptl)	% dev	ref
SiH_4	42.99	5.5	51.47	-2.2	59.2	-5.0	65.88	-9.4	76.71	-9.4	84.51	-8.9	95.47	7.6	29, 45, *66*, 70, 117, *136*, *191*
SiF_4	73.83	0.6	83.14	3.0	89.63	2.9	94.09	4.3	99.43	3.7	102.29	3.4	105.38	0.3	29, *66*, 117, *136*, *191*
SiF_3H	63.70	4.2	73.66	4.3	80.92	2.9	86.19	2.7	93.12	1.7	97.33	1.3	102.59	-1.7	29, *66*, 117, *191*
SiF_3H_2	54.48	9.0	69.71	-2.4	72.58	2.3	78.61	0.4	87.12	-0.9	92.70	-1.4	100.03	3.4	29, *66*, 117
$SiFH_3$	47.39	10.5	57.19	3.5	65.23	0.0	71.78	-3.5	81.66	-4.6	88.43	-4.8	97.67	5.4	29, *66*, 117, 130, *136*, *191*
$SiCl_4$	90.42	0.7	96.79	-0.3	100.37	1.1	102.53	0.7	104.84	1.8	105.97	1.3	107.13	0.1	29, *66*, 70, 117, *136*, *148*, *191*
$SiCl_3H$	75.64	4.0	83.66	1.5	88.85	1.5	92.47	-0.1	97.21	0.2	100.16	-0.4	103.97	-1.6	29, *66*, 70, 117, *191*
$SiCl_2H_2$	62.38	8.3	71.52	2.6	78.03	1.0	82.94	-1.7	89.97	-2.1	94.65	-2.6	100.98	3.3	29, *66*, 70, 117, *136*, *191*
$SiClH_3$	51.29	10.1	60.99	1.5	68.03	-0.7	74.01	-4.6	83.09	-5.2	89.41	-5.4	98.14	5.3	29, *66*, 70, 117 130, *136*, *191*
$SiBr_4$	97.12	3.4	101.32	-0.8	103.55	1.8	104.86	2.3	106.22	4.2	106.88	4.2	107.54	1.0	13, 29, *66*, 117, *136*, *191*
$SiBr_3H$	80.57	1.4	87.16	0.9	91.40	1.9	94.38	1.1	98.40	2.0	100.97	1.8	104.36	0.8	29, *66*, 117, *191*
$SiBr_2H_2$	65.73	5.8	74.01	1.9	79.88	1.2	84.36	-1.0	90.86	-0.8	95.27	-1.2	101.29	2.8	13, 29, *66*, 117, *136*, *191*
$SiBrH_3$	53.05	8.3	62.02	1.4	69.06	-0.8	74.80	-4.3	83.59	-4.5	89.75	-4.7	98.30	-5.1	13, 29, *66*, 117, *136*, *191*
SiI_4	100.65	-3.2	103.61	-0.7	105.13	3.7	106.00	4.6	106.89	9.6	107.31	9.7	107.74	6.8	13, 29, *66*, 117
SiI_3H	84.02	0.4	89.64	0.1	93.23	2.8	95.79	2.4	99.32	5.9	101.63	5.8	104.69	3.5	29
SiI_2H_2	68.15	4.7	75.84	1.0	81.25	1.7	85.40	-0.1	91.51	2.0	95.71	1.7	101.49	0.1	29
$SiIH_3$	54.58	6.9	63.22	0.4	69.98	-0.8	75.51	-4.0	84.06	-3.2	90.08	-3.2	98.46	-3.6	13, 29, *66*, 117, 130, *136*, *191*
$SiFCl_3$	90.23	-5.0	96.33	-2.7	99.87	-0.7	102.08	-0.1	104.51	1.2	105.74	1.2	107.01	-0.4	29
SiF_3Cl	79.57	-2.6	88.26	0.1	93.85	0.7	97.50	1.9	101.69	2.3	103.85	2.2	106.13	-0.6	29
$SiCl_3Br$	92.26	-1.6	98.03	-0.6	101.25	1.2	103.18	1.1	105.23	2.4	106.23	2.0	107.24	0.2	13, 29, *66*, 117, *136*, *191*
$SiCl_2Br_2$	94.01	-2.4	99.20	-0.7	102.09	1.3	103.76	1.5	105.60	2.9	106.48	2.7	107.36	0.4	13, 29, *66*, 117, *136*, *191*
$SiClBr_3$	95.56	-2.9	100.29	-0.8	102.84	1.6	104.35	1.9	105.94	3.6	106.69	3.4	107.45	0.7	13, 29, *66*, 117, *136*, *191*
$SiCl_3I$	93.26	-1.7	98.74	-0.7	101.75	1.6	103.51	1.6	105.44	3.7	106.36	3.4	107.32	1.6	117
$SiClI_3$	98.37	-2.9	102.13	-0.8	104.10	2.9	105.23	3.6	106.44	7.6	107.03	7.6	107.61	5.0	117
$SiBr_3I$	97.86	-3.2	101.88	-0.8	103.93	2.3	105.14	2.9	106.36	5.6	106.98	5.6	-	-	13, *66*, *136*
$Si(CH_3)_4$	143.80	-11.7	172.80	-7.6	199.00	-4.9	219.70	-2.7	255.90	-0.5	283.20	0.6	-	-	13, 29, 45, *66*, 71, 117, *136*, 137, *191*
$Si(CH_3)_3H$	119.80	-11.0	145.20	-8.8	165.70	-5.8	183.50	-4.5	212.10	-1.7	234.80	-0.8	-	-	13, 45, 137, 168, *191*
$Si(CH_3)_2H_2$	92.40	-6.7	112.00	-6.2	129.70	-5.3	144.80	-5.6	168.10	-3.6	186.00	-2.7	-	-	13, 45, *66*, 137, 168, *191*
CH_3SiH_3	66.20	-0.7	81.10	-4.2	93.50	-4.3	104.20	-5.8	121.30	-4.5	134.30	-4.0	-	-	45, *66*, 137, 158, 167, *191*
$Si(OCH_3)_4$	175.73	-1.8	213.38	0.9	242.67	3.9	271.96	4.3	317.98	4.5	351.46	4.3	401.66	1.9	126
CH_3SiF_3	90.34	-3.9	104.77	-0.6	116.18	0.3	125.02	1.6	138.11	2.1	147.23	2.3	160.74	-0.1	13, 29, *66*, 117, *136*, 159
$Si(CH_3)_2F_2$	108.91	-8.0	127.70	-3.9	143.55	-1.9	156.69	-0.5	177.15	1.0	192.46	1.5	-	-	11, 13, *66*, 168
$Si(CH_3)_3F$	123.09	-7.7	146.82	-3.8	167.95	-1.7	187.77	-1.6	214.64	1.0	236.73	1.5	271.42	0.0	13, *66*, 168
CH_3SiCl_3	102.64	-3.5	114.70	-2.1	123.90	-0.4	131.13	-0.2	141.95	1.2	149.84	1.3	162.00	0.0	29, *66*, 71, 117, 159
$C_2H_5SiCl_3$	124.56	-4.1	142.42	-2.0	156.86	-0.1	168.61	0.5	186.86	1.7	200.37	1.7	221.08	0.3	72
$Si(CH_3)_2Cl_2$	117.65	-7.9	135.06	-5.2	149.45	-2.7	161.34	-1.8	180.20	0.3	194.51	0.9	272.09	-20.2	11, 13, 71, 117, *136*, *148*
$Si(CH_3)_3Cl$	129.24	-8.9	152.30	-5.5	172.26	-2.8	189.33	-1.7	216.81	0.4	238.03	1.1	-	-	13, *66*, 71, 117, *136*, 166
$Si(CH_3)_2Br_2$	122.13	-9.6	138.45	-6.0	151.96	-3.0	163.30	-1.7	181.42	0.7	195.35	1.4	-	-	11
$Si(CH_3)_2I_2$	125.19	-10.4	141.17	-7.0	154.18	-3.2	165.06	-1.7	182.67	1.8	196.19	2.6	-	-	11
$Si(CH_3)_2HF$	102.76	-9.3	122.97	-7.4	139.16	-5.3	152.55	-4.1	173.64	-1.8	189.62	-0.8	-	-	11
$Si(CH_3)_2HCl$	106.52	-8.7	126.31	-7.7	142.05	-5.6	154.85	-4.7	175.18	-2.2	190.71	-1.1	-	-	11
$Si(CH_3)_2HBr$	107.28	-8.4	125.85	-6.6	141.08	-4.3	153.85	-3.4	174.35	-1.1	190.04	-0.2	-	-	11
$Si(CH_3)_2HI$	108.45	-8.5	126.98	-6.9	142.09	-4.3	154.72	-3.4	174.97	-0.5	190.46	0.4	-	-	11
Si_2Cl_6	152.21	-4.7	161.80	-6.9	167.19	-5.0	170.41	-6.6	173.89	-4.9	175.56	-4.7	177.32	-0.6	124
Si_2H_6	74.73	-0.4	-	-	104.47	-7.6	-	-	131.96	-8.8	144.05	-8.3	160.29	-7.6	*66*, 137, *191*
Si_3H_8	104.68	-1.1	-	-	149.20	-8.3	-	-	187.23	-8.6	203.72	-8.1	-	-	137
i-Si_4H_{10}	142.17	-6.7	-	-	195.23	-9.3	-	-	242.34	-8.4	263.05	-7.9	-	-	137
neo-Si_5H_{10}	177.65	-15.4	-	-	241.00	-17.2	-	-	297.61	-17.2	322.59	-17.2	-	-	137
$(CH_3)H_2Si_2H_3$	91.25	4.0	-	-	134.77	-3.7	-	-	174.81	-4.7	192.59	-4.4	218.24	-4.8	137
$(CH_3)_2HSi_2H_3$	111.55	3.3	-	-	166.10	-1.8	-	-	217.57	-2.1	240.87	-2.0	275.31	-2.9	137
$(CH_3)_3Si_2H_3$	126.82	7.0	-	-	194.22	1.1	-	-	258.74	0.2	288.07	0.0	331.54	-1.3	137
$(CH_3)H_2Si_2H_2(CH_3)$	110.54	4.3	-	-	166.19	-1.9	-	-	217.74	-2.2	241.00	-2.0	275.39	-2.9	137
$(CH_3)_2HSi_2H(CH_3)_2$	150.54	3.7	-	-	228.49	0.5	-	-	303.05	0.8	337.44	0.8	390.12	-0.8	137
$(CH_3)_3Si_2H_2(CH_3)$	146.06	6.9	-	-	225.60	1.8	-	-	301.62	1.3	336.48	1.1	389.66	-0.7	137
$(CH_3)_3Si_2H(CH_3)_2$	164.98	7.0	-	-	256.02	2.7	-	-	343.97	2.3	384.34	2.0	446.85	-0.1	137
$(CH_3)_3Si_2(CH_3)_3$	179.66	9.6	-	-	283.38	4.5	-	-	384.68	3.5	431.33	3.0	503.63	0.5	137
$Si_2O(CH_3)_6$	244.30	-14.7	295.77	-11.1	336.77	-7.4	370.49	-5.1	424.13	-1.6	465.26	-0.2	530.94	-0.8	13, 123, *136*, 148, 150, *191*
$Si(C_6H_5)_4$	372.38	-5.1	489.53	-3.9	585.76	-2.6	661.07	-2.0	769.86	-1.1	845.17	-0.8	949.77	-0.2	125
$Si(C_6H_5)_3Cl$	301.25	-4.6	389.11	-3.1	460.24	-1.5	518.82	-1.4	602.50	-0.8	656.89	-0.2	740.57	-0.4	125

Table A.5. (Continued)

	300 K		400 K		500 K		600 K		800 K		1000 K		1500 K		
compound	C°_p (exptl)	% dev	C°_p (exptl)	% dev	C°_p (exptl)	% dev	C°_p (exptl)	% dev	C°_p (exptl)	% dev	C°_p (exptl)	% dev	C°_p (exptl)	% dev	ref
$C_6H_5SiCl_3$	158.45	-1.8	192.67	-1.4	219.45	-0.3	240.20	-0.3	269.62	0.3	289.32	0.3	317.40	0.0	125
SiH_3CCH	72.55	-12.6	-	-	-	-	-	-	-	-	-	-	-	-	*191*
SiH_3CN	65.70	-7.3	76.11	1.4	84.34	-1.7	91.14	-1.2	102.57	1.3	109.50	1.2	-	-	97
SiH_3NCS	79.62	-7.8	92.97	-8.6	103.34	-6.5	111.71	-7.8	124.26	-6.5	132.88	-5.2	-	-	149
SiH	30.08	-6.0	30.04	-6.0	30.48	-3.1	31.17	-9.6	32.71	-7.6	34.01	-7.8	36.08	-4.3	29, *66*
SiC_2	45.68	-11.0	48.83	-5.6	51.29	0.7	53.26	-1.1	56.08	2.2	57.87	2.6	60.13	7.2	29, *66*
SiF	32.67	8.0	33.87	9.5	34.84	10.6	35.53	6.4	36.40	6.1	36.89	4.6	37.52	3.2	29, *66*, *191*
SiF_2	44.59	7.6	48.46	9.9	51.11	10.4	52.89	9.5	54.96	9.4	56.05	8.8	57.21	6.3	29, *66*, *191*
SiF_3	59.77	1.5	66.34	4.7	70.84	5.0	73.89	5.5	77.48	5.3	79.37	5.0	81.39	1.9	29, 66
SiCl	35.80	10.0	36.44	9.1	36.83	10.9	37.09	5.4	37.40	5.6	37.59	3.7	37.91	3.5	29, *66*, *191*
$SiCl_2$	51.31	9.5	53.89	8.9	55.30	10.4	56.13	7.8	57.00	8.6	57.42	7.6	57.85	6.9	29, *66*, *191*
$SiCl_3$	70.35	3.7	75.38	2.9	77.88	4.3	79.37	3.2	80.95	4.2	81.72	3.5	82.50	2.3	29, *66*
SiBr	38.75	4.2	39.03	4.5	38.90	7.6	38.74	3.5	38.53	5.1	38.45	4.0	38.52	2.9	29, *66*
BH_3	36.27	-10.6	38.93	-5.8	42.04	-2.7	45.45	-1.7	52.34	-0.1	58.40	0.5	68.60	0.6	29
BF_3	50.59	5.7	57.49	9.9	62.88	8.1	67.05	9.6	72.57	6.8	75.86	5.8	79.59	2.6	29, 88, 129, *191*
BHF_2	42.48	9.3	48.86	11.2	54.50	8.1	59.14	8.0	65.88	4.9	70.34	3.9	76.33	1.4	29
BCl_3	62.76	4.8	68.79	3.6	72.64	3.0	72.27	7.1	78.32	2.4	79.91	2.0	81.66	1.8	29, 88, 129, *191*
$BHCl_2$	49.78	9.8	56.48	5.8	61.45	3.4	65.12	2.1	70.16	1.1	73.43	0.6	77.90	0.7	29
BBr_3	67.94	1.2	72.65	2.2	75.63	2.9	77.57	3.6	79.81	4.3	80.93	4.4	82.11	2.7	29, 88, 132, *191*
$BHBr_2$	53.38	6.1	59.45	3.8	63.80	2.7	66.97	2.3	71.36	2.2	74.26	2.2	78.30	1.2	29
BI_3	70.87	0.8	74.98	1.4	77.41	4.1	78.96	5.2	80.66	9.1	81.52	9.5	82.39	8.2	88, 132, 139, *191*
$BClF_2$	54.59	5.4	61.65	6.8	66.14	6.2	69.78	7.2	74.39	5.4	77.56	4.0	80.28	2.3	29, 129
$BBrF_2$	56.57	3.5	62.74	6.6	67.30	5.9	70.69	7.2	75.07	5.8	77.60	5.2	80.48	2.5	1, 129, *191*
BCl_2F	59.17	4.2	65.34	4.9	70.30	3.2	72.74	4.6	76.54	3.6	78.50	3.3	80.90	2.1	29, 129
BBr_2F	62.44	2.0	67.84	4.0	71.57	4.2	74.22	5.2	77.51	4.9	79.29	4.8	81.32	2.6	1, 129, *191*
$BBrCl_2$	64.56	3.4	70.08	3.1	73.70	2.9	76.07	3.0	78.85	3.0	80.29	2.7	81.82	2.1	1, 29, 129, *191*
BBr_2Cl	66.14	2.4	71.30	2.8	74.63	3.0	76.79	3.4	79.28	3.7	80.59	3.6	81.98	2.4	1, 29, 129, *191*
BF_2OH	52.16	10.9	61.51	10.9	69.37	7.6	75.61	7.6	84.31	5.0	89.89	4.0	97.65	0.4	29
B_2H_6	58.40	2.7	74.26	-2.4	88.68	-5.6	101.33	-7.2	121.66	-7.8	136.39	-7.7	157.55	-7.7	29, *191*
B_2F_4	77.14	-0.6	88.72	4.9	97.54	4.5	104.16	6.9	112.82	5.9	117.81	5.5	123.55	2.3	29
B_2Cl_4	95.06	-2.1	104.80	-0.9	111.31	-0.1	115.68	0.8	120.79	1.9	123.47	1.9	126.37	1.6	29
B_5H_9	94.51	14.9	130.21	4.2	161.37	-1.7	187.61	-4.6	227.37	-6.4	254.40	-7.1	291.07	-8.2	29, *191*
$B_{10}H_{14}$	180.96	4.7	249.95	-3.6	306.43	-7.4	351.66	-8.9	417.19	-8.7	460.36	-8.7	517.82	-9.2	29, *191*
HBO	35.33	-8.2	38.92	-7.9	41.85	-7.2	44.34	-7.1	48.41	-6.0	51.50	-5.5	56.21	-4.2	29
HBS	36.88	-1.4	41.31	-5.8	44.67	-4.8	47.24	-6.9	50.97	-5.0	53.58	-4.5	57.42	-2.9	29
BF	29.61	-5.2	30.58	0.6	31.72	1.4	32.77	1.6	34.36	0.4	35.39	0.2	36.72	1.9	29, *191*
BCl	31.69	1.5	33.34	0.4	34.51	-0.2	35.32	-2.1	36.31	-2.5	36.86	-2.7	37.57	1.0	29, *191*
BBr	32.82	1.0	34.37	0.3	35.36	0.3	36.00	-1.1	36.75	-0.9	37.16	-0.8	37.71	1.6	29, *191*
BO	29.20	-8.4	29.57	-3.7	30.25	-1.0	31.08	-1.3	32.68	-0.8	33.93	-1.4	35.74	0.5	29
BN	29.46	-7.5	30.28	-5.7	31.33	-3.4	32.36	-5.8	34.00	-4.7	35.11	-4.7	36.63	-0.5	29, *191*
BS	30.07	2.0	31.38	0.6	32.63	3.1	33.66	-0.5	35.06	0.7	35.90	0.2	36.93	2.4	29
BF_2	40.63	0.3	44.41	5.8	47.49	5.4	49.83	7.1	52.84	6.0	54.54	6.1	56.46	5.4	29
BCl_2	47.46	3.2	50.92	2.8	53.07	3.0	54.44	2.8	55.96	3.3	56.73	3.4	57.55	5.2	29
BO_2	43.36	-12.0	47.50	-10.8	50.78	-10.1	53.26	-9.5	56.49	-8.3	58.33	-7.6	60.44	-6.5	29
HBO_2	42.33	3.6	47.55	4.6	52.16	4.6	56.07	4.7	62.14	4.5	66.51	3.8	73.33	1.5	29, *191*
B_2O_3	59.55	0.9	69.53	0.6	76.77	0.9	82.26	1.5	90.15	1.7	95.10	0.8	101.43	-1.6	29, 133
B_2S_3	80.49	-10.8	87.48	-9.4	92.21	-4.0	95.68	-4.0	100.08	0.3	102.59	0.8	105.43	0.1	133
H_3BO_3	65.56	1.6	76.86	2.0	86.36	1.9	94.02	3.4	105.50	4.7	113.80	5.3	126.76	3.2	29
B_2O_2	57.42	-15.3	62.87	-10.8	66.72	-7.4	69.82	-5.5	74.58	-3.0	77.87	-3.1	82.35	-3.8	29
$(BOF)_3$	115.44	-5.9	135.79	-2.6	151.57	-2.9	163.45	-1.1	179.00	-1.3	187.97	-1.8	198.30	-4.8	29
$(BOH)_3$	88.20	-0.6	107.75	-1.8	124.29	-3.3	137.74	-3.6	157.38	-3.7	170.42	-4.3	187.95	-6.2	29
KBO_2	59.13	-2.5	63.99	-1.3	67.60	-0.4	70.39	-0.1	74.30	0.7	76.78	0.5	79.91	-0.1	29
$LiBO_2$	57.37	0.5	62.82	0.5	66.76	0.9	69.74	0.8	73.88	1.3	76.48	0.9	76.76	0.1	29
$NaBO_2$	58.35	-1.2	63.50	-0.5	67.26	0.1	70.13	0.2	74.13	0.9	76.66	0.7	76.86	0.0	29
$B(CH_3)_3$	88.49	5.9	-	-	-	-	-	-	-	-	-	-	-	-	*191*
$BH(OCH_3)_2$	87.91	9.3	-	-	-	-	-	-	-	-	-	-	-	-	*191*
BH_3CO	59.45	-11.1	-	-	-	-	-	-	-	-	-	-	-	-	*191*
$B(CH_3)_3NBH_3$	127.95	-4.1	-	-	-	-	-	-	-	-	-	-	-	-	*191*
$(CH_3)_2NB_2H_5$	117.73	0.6	153.39	1.3	184.40	-5.0	210.09	-5.4	249.67	-5.0	278.02	-4.5	320.00	-5.1	111
AlF_3	62.61	-4.9	68.53	0.1	72.46	0.5	75.14	4.1	78.21	3.6	79.86	4.1	81.6	2.9	151, *191*
$AlCl_3$	71.59	0.4	75.73	1.2	78.12	2.1	79.50	3.3	81.00	3.3	81.76	3.2	-	-	41, 109
$AlBr_3$	75.44	-0.8	78.37	1.7	79.91	3.6	80.83	5.3	81.63	6.2	82.26	6.2	-	-	41, 194
AlI_3	77.14	0.5	79.48	2.5	80.71	5.9	81.41	7.8	82.15	11.4	82.50	11.7	82.86	10.3	29, *191*
$AlCl_2Br$	72.93	0.1	76.65	1.3	78.74	2.5	79.96	3.9	81.30	4.2	81.92	4.2	-	-	40
$AlClBr_2$	74.18	-0.4	77.49	1.5	79.33	3.1	80.41	4.6	81.55	5.1	82.09	5.2	-	-	40
Al_2F_6	133.11	-14.2	148.72	-8.4	158.53	-6.9	164.86	-2.3	172.04	-1.5	175.72	-0.5	179.61	-2.4	29, *191*
Al_2Cl_6	156.89	-11.5	166.71	-8.5	172.00	-6.2	175.12	-3.6	178.40	-2.0	179.99	-1.5	181.60	-1.9	38
Al_2Br_6	168.62	-14.1	174.05	-9.0	176.98	-5.4	178.66	-2.2	180.75	0.1	181.59	0.9	182.42	-1.0	194
Al_2I_6	172.07	-12.7	176.48	-8.2	178.69	-3.3	179.94	0.1	181.22	5.1	181.82	6.1	182.43	4.3	29
Al_2O_2	67.31	-9.6	73.05	-8.5	76.27	-6.2	78.20	-3.6	80.26	-1.2	81.27	0.0	82.30	1.9	29, *191*
AlH	29.38	-7.6	30.04	-9.0	31.00	-9.5	32.01	-11.3	33.75	-12.3	35.02	-11.0	36.84	-3.6	29, *191*
AlI	36.14	11.1	36.78	10.0	37.12	11.1	37.33	10.3	37.60	10.4	37.78	9.5	38.11	10.8	29, *191*
AlN	32.40	3.0	34.02	-0.2	35.09	0.2	35.81	-1.7	36.66	-2.0	37.15	-2.1	37.80	2.5	29
AlO	30.91	6.3	32.49	4.2	33.75	3.3	34.69	2.0	36.00	-0.3	37.21	-2.3	41.28	-7.4	29, *191*
AlS	33.43	10.0	34.87	6.0	35.75	7.8	36.35	5.1	37.42	3.7	38.88	0.0	43.71	-8.2	29, *191*
OAlH	34.67	11.2	39.92	3.3	44.49	-1.7	48.09	-4.6	52.95	-7.4	55.82	-7.6	59.19	-5.2	29
OAlOH	50.27	-0.6	56.42	-2.3	60.95	-2.5	64.27	-1.4	68.77	-0.5	71.77	0.3	76.34	0.5	29
Al_2O	45.75	8.1	49.13	7.8	51.53	8.4	53.18	8.9	55.09	8.7	56.12	8.5	57.22	10.5	29, 131, *191*

Table A.5. (Continued)

compound	300 K		400 K		500 K		600 K		800 K		1000 K		1500 K		ref
	C°_p (exptl)	% dev	C°_p (exptl)	% dev	C°_p (exptl)	% dev	C°_p (exptl)	% dev	C°_p (exptl)	% dev	C°_p (exptl)	% dev	C°_p (exptl)	% dev	
AlO_2	49.97	-11.4	53.58	-10.9	56.00	-9.7	57.61	-8.2	59.47	-7.0	60.44	-6.1	61.47	-4.3	29
$LiAlF_4$	93.89	-2.3	105.76	-0.2	113.44	-0.9	118.47	1.6	124.24	1.0	127.20	1.3	130.35	-0.8	37
$Al(CH_3)_3$	80.33	24.2	-	-	-	-	-	-	-	-	-	-	-	-	122
$Al_2(CH_3)_6$	140.16	38.9	-	-	-	-	-	-	-	-	-	-	-	-	16, 187
$NaAlF_4$	106.00	-13.4	-	-	-	-	-	-	-	-	-	-	-	-	98
av % dev		6.2		4.2		3.8		3.8		3.8		3.6		2.8	
% bias		-0.4		-0.6		-0.4		-0.5		-0.3		-0.2		-0.3	

[a] All C°_p are in kJ mol^{-1} K^{-1}. Underlined reference numbers indicate references from which the accepted values were taken. Italic reference numbers indicate where only one heat capacity value at 298.15 K is available.

Table A.6. Predictions of the Ideal Gas Entropy at 298.15 K for Silicon Compounds[a,b]

compound	exptl S°_{298}	extended Benson		O'Neal and Ring		Van Dalen–Van den Berg		ref
		S°_{298}	% dev	S°_{298}	% dev	S°_{298}	% dev	
SiH_4	204.1	207.5	1.7	208.6	2.2	204.6	0.2	29, 45, 66, 70, 117, 137, 191
SiF_4	282.7	286.9	1.5	285.6	1.0	-	-	29, 36, 66, 117, 137, 191
SiF_3H	277.3	278.6	0.5	277.9	0.2	-	-	29, 117, 191
SiF_2H_2	262.1	262.1	0.0	262.0	0.0	-	-	29, 117
$SiFH_3$	238.4	238.9	0.2	239.4	0.4	-	-	29, 66, 117, 130, 137, 191
$SiCl_4$	330.8	335.9	1.6	331.3	0.2	330.8	0.0	29, 66, 70, 117, 137, 191
$SiCl_3H$	313.8	315.4	0.5	312.2	0.5	313.1	0.2	29, 66, 70, 117, 191
$SiCl_2H_2$	285.8	286.6	0.3	284.9	0.3	286.5	0.2	29, 66, 70, 117, 137, 191
$SiClH_3$	250.5	251.2	0.3	250.8	0.1	251.5	0.4	29, 70, 117, 130, 137, 191
$SiBr_4$	377.6	378.2	0.2	377.7	0.0	-	-	29, 66, 117, 137, 191
$SiBr_3H$	348.0	347.0	0.3	346.9	0.3	-	-	29, 66, 117, 191
$SiBr_2H_2$	310.1	307.8	0.8	308.0	0.7	-	-	29, 66, 117, 137, 191
$SiBrH_3$	262.5	261.7	0.3	262.4	0.0	-	-	29, 66, 117, 137
SiI_4	416.4	415.5	0.2	422.8	1.6	-	-	29, 66, 117
SiI_3H	375.0	375.0	0.0	380.8	1.6	-	-	29
$SiIH_3$	271.0	271.1	0.0	273.7	1.0	-	-	29, 66, 130, 137, 191
$SiFCl_3$	366.1	335.2	8.4	331.4	9.5	-	-	29
SiF_3Cl	308.7	310.7	0.6	308.6	0.1	-	-	29
$SiCl_3Br$	353.5	358.0	1.3	354.4	0.3	-	-	66, 117, 137
$SiCl_2Br_2$	370.0	372.0	0.5	369.4	0.2	-	-	66, 117, 137, 191
$SiClBr_3$	376.5	379.1	0.7	377.6	0.3	-	-	66, 117, 137, 191
$SiCl_3I$	363.0	367.4	1.2	365.7	0.8	-	-	117
$SiClI_3$	405.2	407.1	0.5	411.5	1.6	-	-	117
$SiBr_3I$	400.5	399.0	0.4	400.5	0.0	-	-	66, 137
$Si(CH_3)_4$	356.7	356.6	0.0	358.9	0.6	357.6	0.3	29, 45, 66, 71, 117, 136, 137, 150, 191
$(CH_3)_3SiH$	332.5	330.9	0.5	332.8	0.1	331.9	0.2	45, 66, 136, 168, 191
$(CH_3)_2SiH_2$	300.6	297.0	1.2	298.6	0.6	297.5	1.0	45, 66, 136, 168, 191
CH_3SiH_3	256.1	256.3	0.1	257.7	0.6	255.7	0.2	45, 66, 136, 158, 191
$Si(CH_3)F_3$	315.5	315.9	0.1	315.4	0.0	-	-	29, 66, 71, 159
$Si(CH_3)_2F_2$	335.6	336.6	0.3	337.1	0.5	-	-	11, 66, 168
$Si(CH_3)_3F$	350.7	350.7	0.0	352.1	0.4	-	-	66, 137, 168
$Si(C_2H_5)Cl_3$	392.4	392.0	0.1	389.0	0.8	392.4	0.0	72
$Si(CH_3)Cl_3$	351.3	352.6	0.4	349.7	0.5	349.5	0.5	29, 66, 71, 117, 159
$Si(CH_3)_2Cl_2$	359.5	361.2	0.5	360.0	0.1	359.8	0.1	11, 71, 117, 137
$Si(CH_3)_3Cl$	359.4	363.0	1.0	363.5	1.1	363.0	1.0	71, 117, 137, 166, 191
$Si(CH_3)_2Br_2$	384.1	382.3	0.5	383.2	0.2	-	-	11
$Si(CH_3)_2I_2$	403.4	400.9	0.6	405.8	0.6	-	-	11
$Si(CH_3)_2HF$	321.0	322.6	0.5	323.6	0.8	-	-	11
$Si(CH_3)_2HCl$	332.3	334.8	0.8	335.1	0.8	335.3	0.9	11, 137
$Si(CH_3)_2HBr$	345.9	345.4	0.2	346.7	0.2	-	-	11
$Si(CH_3)_2HI$	353.9	354.7	0.0	358.0	1.1	-	-	11
$(CH_3)SiH_2F$	286.7	285.3	0.5	286.1	0.2	-	-	11
$(CH_3)SiH_2Cl$	298.3	297.6	0.2	297.5	0.3	289.2	0.4	11
$(CH_3)SiH_2Br$	310.2	308.1	0.7	309.1	0.4	-	-	11
$(CH_3)SiH_2I$	318.7	317.5	0.4	320.4	0.5	-	-	11
Si_2OF_6	382.7	378.8	1.0	425.0	11.0	-	-	155
Si_2Cl_6	479.4	462.9	3.4	-	-	-	-	124
Si_2H_6	271.5	270.3	0.5	-	-	-	-	66, 136, 191
Si_3H_8	341.8	336.4	1.6	-	-	-	-	136
i-Si_4H_{10}	399.7	390.0	2.4	-	-	-	-	136
neo-Si_5H_{10}	451.0	435.5	3.4	-	-	-	-	136
$(CH_3)H_2SiSiH_3$	318.4	322.5	1.3	-	-	-	-	136
$(CH_3)_2HSiSiH_3$	353.7	359.7	1.7	-	-	-	-	136
$(CH_3)_3SiSiH_3$	372.5	387.9	4.1	-	-	-	-	136
$(CH_3)H_2SiSiH_2(CH_3)$	358.8	363.1	1.2	-	-	-	-	136
$(CH_3)_2HSiSiH_2(CH_3)$	397.7	406.1	2.1	-	-	-	-	136
$(CH_3)_2HSiSiH(CH_3)_2$	427.0	437.6	2.5	-	-	-	-	136
$(CH_3)_3SiSiH_2(CH_3)$	417.1	434.3	4.1	-	-	-	-	136

Table A.6. (Continued)

compound	exptl	extended Benson		O'Neal and Ring		Van Dalen–Van den Berg		ref
	$S°_{298}$	$S°_{298}$	% dev	$S°_{298}$	% dev	$S°_{298}$	% dev	
$(CH_3)_3SiSiH(CH_3)_2$	452.3	471.5	4.3	-	-	-	-	136
$(CH_3)_3SiSi(CH_3)_3$	466.6	493.9	5.8	-	-	-	-	136
$(OC_2H_5)_4Si$	535.6	540.3	0.9	502.8	6.1	-	-	126
$Si_2O(CH_3)_6$	532.1	483.3	9.2	534.9	0.5	-	-	73, 123, 137, 150, 191
$Si(C_6H_5)_4$	648.5	643.7	0.7	-	-	626.4	3.4	125
$Si(C_6H_5)_3Cl$	573.2	578.3	0.9	-	-	558.2	2.6	125
$Si(C_6H_5)Cl_3$	420.8	424.4	0.9	-	-	420.8	0.0	69
SiH_3CCH	269.4	269.4	*	-	-	-	-	66, 191
SiH_3CN	266.3	266.3	*	-	-	-	-	66, 97
SiH_3NCS	309.9	309.9	*	-	-	-	-	66, 149
av % dev		1.3		1.1		0.6		
% bias		0.1		0.2		-0.1		

[a] All $S°_{298}$ are in J mol^{-1} K^{-1}, and deviations are absolute. Accepted references are underlined. [b] Asterisks designate compounds from which a contribution value has been directly derived. The percentage deviation would then, of course, be zero.

Table A.7. Predictions of the Ideal Gas Entropy at 298.15 K for Boron Compounds[a,b]

compound	exptl	extended Benson		ref	compound	exptl	extended Benson		ref
	$S°_{298}$	$S°_{298}$	% dev			$S°_{298}$	$S°_{298}$	% dev	
BF_3	254.6	250.6	1.6	29, 36, 88, 129, 191	BBr_2F	310.2	314.2	1.3	1, 29, 129, 191
BHF_2	244.0	244.6	0.2	29	$BBrCl_2$	310.8	312.0	0.4	1, 29, 129, 191
BCl_3	289.9	283.8	2.1	29, 88, 129, 191	BBr_2Cl	322.1	325.3	1.0	1, 29, 129, 191
$BHCl_2$	268.3	266.7	0.6	29	BF_2OH	269.2	265.7	1.3	29
BBr_3	330.3	323.7	2.0	29, 88, 132	B_2F_4	318.5	316.6	0.6	29, 191
$BHBr_2$	292.3	293.3	0.4	29	B_2Cl_4	358.9	360.8	0.5	29, 191
BI_3	349.4	349.4	*	29, 88, 132, 139, 191	$B(CH_3)_3$	314.6	316.3	0.6	191
$BClF_2$	272.8	276.5	1.4	29, 129, 191	$B(C_2H_5)_3$	437.6	434.3	0.8	191
$BBrF_2$	287.5	289.8	0.8	1, 29, 129, 191	$HB(OCH_3)_2$	323.8	327.9	1.3	191
BCl_2F	285.2	287.6	0.8	29, 129, 191	$B(OCH_3)_3$	384.9	375.5	2.4	191
					av % dev			1.1	
					% bias			-0.1	

[a] All $S°_{298}$ are in J mol^{-1} K^{-1}, and deviations are absolute. Accepted references are underlined. [b] Asterisks designate compounds from which a contribution value has been directly derived. The percentage deviation would then, of course, be zero.

Table A.8. Predictions of Critical Temperatures for Silicon Compounds[a–c]

compound	exptl		Lyderson		revised Lyderson		extended Ambrose		ref
	T_b	T_c	T_c	% dev	T_c	% dev	T_c	% dev	
SiF_4	187.2	259.0	284.2	9.7	285.6	10.3	296.7	14.5	4, 5, 112, 157
$SiCl_4$	330.8	508.1	504.7	0.7	507.2	0.2	530.7	4.4	4, 5, 112, 135, 157
$SiCl_3H$	285.4	438.6	-	-	439.3	0.2	441.1	0.6	4, 5, 112, 135, 157
$SiBr_4$	427.1	663.1	675.7	1.9	679.4	2.5	685.2	3.3	4, 5, 112, 135, 157
$SiBr_3H$	382.1	610.0	-	-	604.5	0.9	590.6	3.2	4, 5, 112, 135, 157
SiI_4	560.5	944.0	877.3	7.1	881.9	6.6	899.2	4.7	4, 5
$SiFCl_3$	285.4	438.6	434.9	0.8	437.1	0.3	452.3	3.1	4, 5, 112, 157
SiF_2Cl_2	240.9	369.0	366.7	0.6	368.5	0.1	381.8	3.5	4, 5, 112, 157
SiF_3Cl	203.1	307.7	308.8	0.3	310.3	0.8	321.9	4.6	4, 5, 112, 157
$SiCl_3Br$	353.5	540.0	544.1	0.8	546.8	1.3	567.1	5.0	162
$SiCl_2Br_2$	377.5	585.0	586.2	0.2	589.3	0.7	605.6	3.5	162
$SiClBr_3$	401.0	618.0	628.5	1.7	631.8	2.2	643.3	4.1	162
CH_3SiH_3	215.6	352.5	-	-	352.5	*	352.5	*	4, 5, 157
$Si(CH_3)_4$	299.8	448.6	450.9	0.5	453.0	1.0	455.0	1.4	4, 5, 82, 114, 115, 157
$Si(C_2H_5)_4$	427.9	603.7	593.6	1.7	595.6	1.3	600.2	0.6	4, 5, 61, 81, 157
$Si(OCH_3)_4$	394.7	562.8	545.6	3.0	547.5	2.7	535.1	4.9	5, 157, 193
$Si(OC_2H_5)_4$	438.7	592.2	572.8	3.3	574.1	3.0	569.1	3.9	5, 157, 193
$Si(OC_3H_7)_4$	502.0	647.7	630.9	2.6	631.8	2.4	630.2	2.7	5, 157, 193
CH_3SiCl_3	338.8	517.4	515.1	0.5	517.6	0.0	533.7	3.2	5, 157, 165, 171
$(CH_3)_2SiCl_2$	343.5	520.4	520.3	0.0	522.8	0.5	532.1	2.3	4, 5, 157, 172
$(CH_3)_3SiCl$	333.2	497.8	502.9	1.0	505.3	1.5	508.2	2.1	4, 5, 157, 172
CH_3SiH_2Cl	280.0	517.8	-	-	517.8	*	517.8	*	4, 5, 157
$C_2H_5SiCl_3$	371.6	560.0	551.9	1.5	554.4	1.0	569.7	1.7	4, 5, 157, 172
$(C_2H_5)_2SiCl_2$	403.6	595.8	584.7	1.9	587.1	1.5	596.1	0.0	4, 5, 157, 171
$H_2C[Si(CH_3)_3]_2$	407.0	573.9	559.8	2.5	563.6	1.8	570.8	0.5	5, 116
$Si(CH_3)_3]_2O$	372.7	516.6	512.2	0.8	525.8	1.8	530.2	2.6	4, 5, 42, 157, 201, 202, 203
$Si_3(CH_3)_8O_2$	425.0	562.9	549.3	2.4	568.7	1.0	576.7	2.4	4, 5, 42, 61, 157, 201
$Si_4(CH_3)_{10}O_3$	465.0	599.4	578.9	3.4	598.1	0.2	608.7	1.5	4, 5, 42, 61, 157, 201

Table A.8. (Continued)

	exptl		Lyderson		revised Lyderson		extended Ambrose		
compound	T_b	T_c	T_c	% dev	T_c	% dev	T_c	% dev	ref
$Si_5(CH_3)_{12}O_4$	502.0	629.0	615.0	2.2	621.2	1.2	629.2	0.0	4, 5, 61, 157, 201
$Si_4(CH_3)_{10}O_3$	465.0	599.4	578.9	3.4	598.1	0.2	608.7	1.5	4, 5, 42, 61, 157, 201
$Si_5(CH_3)_{12}O_4$	502.0	629.0	615.0	2.2	621.2	1.2	629.2	0.0	4, 5, 61, 157, 201
$Si_6(CH_3)_{14}O_5$	536.0	653.2	659.5	1.0	659.9	1.0	666.5	2.0	4, 5, 61, 157, 201
$Si_7(CH_3)_{16}O_6$	561.0	671.8	707.7	5.3	686.7	2.2	684.5	1.9	4, 5, 61, 157, 201
$Si_8(CH_3)_{18}O_7$	584.0	688.9	772.5	12.1	718.1	4.2	701.3	1.8	4, 5, 61, 157, 201
$HSi_3(CH_3)_7O_2$	415.8	553.4	-	-	558.8	1.0	559.3	1.1	128
$CH_3Si[OSi(CH_3)_3]_3$	464.7	597.0	578.5	3.1	597.8	0.1	608.3	1.9	61
$Si[OSi(CH_3)_3]_4$	494.9	623.2	606.3	2.7	619.4	0.6	629.7	1.0	61
$Si_2(C_2H_5)_6O$	504.0	693.0	642.1	7.3	651.7	6.0	661.7	4.5	4, 5
$Si_4(C_2H_5)_{10}O_3$	598.0	788.0	738.2	6.3	731.9	7.1	727.5	7.7	4, 5
$Si_5(C_2H_5)_{12}O_4$	633.0	823.0	820.8	0.3	785.6	4.5	751.8	8.7	4, 5
$[(CH_3)_2SiO]_3$	409.6	554.2	542.2	2.2	562.9	1.6	575.9	3.9	61
$[(CH_3)_2SiO]_4$	448.0	586.5	567.0	3.3	587.0	0.1	604.1	3.0	4, 5, 202, 203
$[(CH_3)_2SiO]_5$	483.0	617.4	595.9	3.5	611.6	0.9	630.4	2.1	4, 5
$[(C_2H_5)_2SiO]_3$	520.0	673.0	649.5	3.5	662.5	1.6	678.0	0.7	4, 5
$[(C_2H_5)_2SiO]_4$	569.0	698.0	696.5	0.2	700.9	0.4	712.2	2.0	4, 5
				Overall					
av % dev				2.68		1.92		3.10	
% bias				-0.79		-0.24		1.08	
				Siloxanes					
av % dev				3.50		1.98		2.72	
% bias				-1.37		-0.48		0.41	

[a] All T_b and T_c are in kelvin, and deviations are absolute. Accepted references are underlined. [b] Asterisks designate compounds from which a group contribution was directly derived. The percentage deviation is zero. [c] Dashes indicate compounds for which a value cannot be determined because of missing groups.

Table A.9. Predictions of Critical Pressure for Silicon Compounds[a,b]

		Lyderson		revised Lyderson		extended Ambrose		
compound	exptl P_c	P_c	% dev	P_c	% dev	P_c	% dev	ref
SiF_4	3.720	3.343	10.1	3.632	2.4	3.636	2.3	4, 5, 112
$SiCl_4$	3.593	3.690	2.7	3.949	9.9	3.957	10.1	4, 5
$SiCl_3H$	4.170	-	-	4.175	0.1	4.181	0.3	99, 112
$SiFCl_3$	3.580	3.650	1.9	3.918	9.4	3.926	9.7	4, 5
SiF_2Cl_2	3.500	3.584	2.4	3.861	10.3	3.868	10.5	4, 5
SiF_3Cl	3.460	3.485	0.7	3.769	8.9	3.774	9.1	4, 5
$Si(CH_3)_4$	2.821	2.976	0.9	3.036	7.6	3.039	7.7	4, 5, 82, 114
$Si(C_2H_5)_4$	2.602	2.012	22.7	2.124	18.4	2.122	18.4	4, 5, 81
$Si(OCH_3)_4$	2.873	2.616	8.9	2.779	3.3	2.770	3.6	5, 193
$Si(OC_2H_5)_4$	2.045	1.897	7.2	1.981	3.1	1.975	3.4	5, 193
$Si(OC_3H_7)_4$	1.696	1.488	12.3	1.539	9.2	1.534	9.6	5, 193
CH_3SiCl_3	3.430	3.545	3.4	3.806	10.9	3.813	11.2	4, 5, 157, 165
$(CH_3)_2SiCl_2$	3.490	3.356	3.8	3.615	3.6	3.621	3.7	4, 5, 172
$(CH_3)_3SiCl$	3.200	3.111	2.8	3.364	5.1	3.368	5.3	4, 5, 172
$C_2H_5SiCl_3$	3.330	3.148	5.5	3.356	0.8	3.360	0.9	4, 5, 172
$(C_2H_5)_2SiCl_2$	3.060	2.701	11.7	2.868	6.3	2.869	6.2	4, 5
$H_2C[Si(CH_3)_3]_2$	1.990	1.795	9.8	1.980	0.5	1.985	0.3	5, 116
$[Si(CH_3)_3]_2O$	1.910	1.901	0.5	1.956	2.4	1.956	2.4	4, 5, 42, 201, 202
$Si_3(CH_3)_8O_2$	1.420	1.429	0.6	1.437	1.2	1.436	1.2	4, 5, 42, 201
$Si_4(CH_3)_{10}O_3$	1.150	1.142	0.7	1.134	1.4	1.134	1.4	4, 5, 42, 201
$Si_5(CH_3)_{12}O_4$	0.950	0.951	0.1	0.937	1.4	0.936	1.5	4, 5, 201
$Si_6(CH_3)_{14}O_5$	0.800	0.814	1.8	0.798	0.3	0.797	0.4	4, 5, 201
$Si_7(CH_3)_{16}O_6$	0.680	0.712	4.7	0.694	2.1	0.694	2.1	4, 5, 201
$Si_8(CH_3)_{18}O_7$	0.620	0.632	2.0	0.615	0.8	0.614	0.9	4, 2, 201
$HSi_3(CH_3)_7O_2$	1.481	-	-	1.481	0.0	1.480	0.1	128
$[(CH_3)_2SiO]_4$	1.340	1.307	2.5	1.289	3.8	1.288	3.9	4, 5, 81, 116, 203
$[(CH_3)_2SiO]_5$	1.035	1.076	3.9	1.061	2.5	1.060	2.4	5, 116
				Overall				
av % dev			4.94		4.66		4.76	
% bias			-2.68		0.90		0.91	
				Siloxanes				
av % dev			1.87		1.59		1.62	
% bias			1.24		0.06		-0.01	

[a] All P_c are in megapascals, and deviations are absolute. Accepted references are underlined. [b] Dashes indicate compounds for which a value cannot be determined because of missing groups.

Table A.10. Prediction of the Critical Volume for Silicon Compounds[a]

compound	exptl V_c	pred V_c	% dev	ref	compound	exptl V_c	pred V_c	% dev	ref
$SiCl_4$	0.326	0.324	0.6	4, 5, 99, 112, 135, 135	$C_2H_5SiCl_3$	0.403	0.386	4.2	4, 5, 157, 172
$SiCl_3H$	0.268	0.280	4.6	4, 99, 135	$(C_2H_5)_2SiCl_2$	0.455	0.448	1.6	4, 5, 157, 171
$SiBr_4$	0.382	0.400	4.7	4, 5, 99, 135	$H_2C[Si(CH_3)_3]_2$	0.644	0.623	3.2	5
$SiBr_3H$	0.305	0.337	10.6	4, 5, 99, 135	$[Si(CH_3)_3]_2O$	0.629	0.672	6.8	4, 5, 42, 61, 115, 116, 157
SiI_4	0.558	0.498	10.7	4, 5	$Si_3(CH_3)_8O_2$	0.906	0.942	4.0	4, 5, 42, 61, 115, 157
$SiCl_3Br$	0.346	0.343	0.9	162	$Si_4(CH_3)_{10}O_3$	1.209	1.213	0.3	4, 5, 42, 61, 115, 157
$SiCl_2Br_2$	0.364	0.362	0.6	162	$Si_5(CH_3)_{12}O_4$	1.509	1.483	1.7	4, 5, 61, 115, 157
$SiClBr_3$	0.384	0.381	0.8	162	$Si_6(CH_3)_{14}O_5$	1.807	1.754	2.9	4, 5, 61, 115
$Si(CH_3)_4$	0.362	0.361	0.4	4, 5, 61, 82, 114, 157	$Si_7(CH_3)_{16}O_6$	2.133	2.025	5.1	4, 5, 61, 115, 157
$Si(C_2H_5)_4$	0.495	0.572	16.2	81, 157	$Si_8(CH_3)_{18}O_7$	2.469	2.295	7.0	4, 5, 61, 115, 157
$Si(OCH_3)_4$	0.445	0.442	0.7	5, 157	$CH_3Si[OSi(CH_3)_3]_3$	1.125	1.213	7.8	61
$Si(OC_2H_5)_4$	0.651	0.653	0.3	5, 157	$Si[OSi(CH_3)_3]_4$	1.400	1.357	3.1	61
$Si(OC_3H_7)_4$	0.853	0.864	1.3	5, 157, 193	$[(CH_3)_2SiO]_3$	0.707	0.743	5.1	61
CH_3SiCl_3	0.348	0.333	4.1	4, 157, 165, 171	$[(CH_3)_2SiO]_4$	0.985	0.982	0.3	5, 61, 81, 82, 116, 157, 203
$(CH_3)_2SiCl_2$	0.350	0.342	2.2	4, 5, 157, 172	$[(CH_3)_2SiO]_5$	1.287	1.220	5.2	5, 61, 116
$(CH_3)_3SiCl$	0.366	0.351	4.0	4, 5, 157, 172					
					Overall				
			av % dev					6.17	
			% bias					0.07	
					Siloxanes				
			av % dev					3.90	
			% bias					-0.11	

[a] All V_c are in cubic meters per kilomole, and deviations are absolute. Accepted references are underlined.

Table A.11. Predictions of the Thermal Conductivity *k* for Silicon Compounds[a]

compound	T_b/K	T_c/K	T/K	exptl $k/(10^{-1}\ W\ m^{-1}\ K^{-1})$	pred $k/(10^{-1}\ W\ m^{-1}\ K^{-1})$	% dev	ref
$Si(OCH_3)_4$	394.7	562.8	283	1.626	1.525	6.2	87
			293	1.609	1.496	7.0	
			313	1.557	1.437	7.7	
			333	1.486	1.377	7.3	
			353	1.436	1.318	8.2	
			363	1.409	1.287	8.6	
$Si(OC_2H_5)_4$	438.7	592.2	260	1.443	1.572	8.9	87
			273	1.419	1.538	8.4	
			293	1.359	1.481	8.9	
			313	1.316	1.426	8.4	
			333	1.269	1.372	8.1	
			353	1.218	1.318	8.2	
			363	1.199	1.291	7.7	
$Si(OC_3H_7)_4$	502.0	647.7	303	1.542	1.567	1.6	2
			323	1.518	1.515	0.2	
			343	1.472	1.464	0.5	
			363	1.441	1.414	1.9	
			383	1.396	1.363	2.4	
			403	1.358	1.312	3.4	
			423	1.320	1.260	4.6	
			443	1.278	1.206	5.6	
			463	1.240	1.152	7.1	
$Si(O\text{-}iC_3H_7)_4$	461.2	*588.4*	303	1.534	1.366	10.9	2
			323	1.512	1.315	13.0	
			343	1.470	1.264	14.0	
			363	1.439	1.212	15.8	
			383	1.390	1.160	16.6	
			403	1.350	1.106	18.1	
			423	1.317	1.050	20.2	
			443	1.271	0.993	21.9	
			463	1.234	0.931	24.5	
$Si(OC_4H_9)_4$	550.7	*678.1*	303	1.568	1.612	2.8	2
			323	1.544	1.562	1.2	
			343	1.519	1.513	0.4	
			363	1.492	1.464	1.9	
			383	1.455	1.415	2.7	
			403	1.409	1.366	3.0	
			423	1.369	1.317	3.8	
			443	1.318	1.267	3.9	
			463	1.274	1.216	4.6	
$Si(O\text{-}iC_4H_9)_4$	531.7	*659.2*	303	1.564	1.534	1.9	2
			323	1.547	1.485	4.0	
			343	1.528	1.436	6.0	
			363	1.480	1.388	6.2	
			383	1.448	1.339	7.5	

Table A.11. (Continued)

compound	T_b/K	T_c/K	T/K	exptl k/(10^{-1} W m^{-1} K^{-1})	pred k/(10^{-1} W m^{-1} K^{-1})	% dev	ref
Si(O-iC_4H_9)$_4$	531.7	*659.2*	403	1.407	1.290	8.3	
			423	1.367	1.241	9.2	
			443	1.314	1.191	9.4	
			463	1.270	1.139	10.3	
Si(O-sC_4H_9)$_4$	525.2	*651.1*	303	1.556	1.505	3.3	2
			323	1.540	1.456	5.4	
			343	1.524	1.408	7.6	
			363	1.481	1.359	8.2	
			383	1.452	1.311	9.7	
			403	1.403	1.262	10.0	
			423	1.364	1.213	11.1	
			443	1.309	1.162	11.2	
			463	1.268	1.110	12.5	
Si(OC_5H_{11})$_4$	615.2	*753.1*	303	1.579	1.751	10.9	2
			323	1.552	1.703	9.7	
			343	1.534	1.656	7.9	
			363	1.492	1.609	7.9	
			383	1.464	1.563	6.8	
			403	1.426	1.518	6.4	
			423	1.374	1.472	7.2	
			443	1.326	1.427	7.6	
			463	1.292	1.381	6.9	
Si(O-iC_5H_{11})$_4$	598.2	*732.6*	303	1.569	1.681	7.1	2
			323	1.544	1.633	5.8	
			343	1.530	1.587	3.7	
			363	1.494	1.541	3.1	
			383	1.462	1.495	2.3	
			403	1.426	1.449	1.6	
			423	1.370	1.404	2.5	
			443	1.330	1.358	2.1	
			463	1.280	1.312	2.5	
Si(O-sC_5H_{11})$_4$	576.2	*705.7*	303	1.572	1.591	1.2	2
			323	1.546	1.544	0.2	
			343	1.532	1.497	2.3	
			363	1.490	1.452	2.6	
			383	1.459	1.406	3.6	
			403	1.420	1.361	4.2	
			423	1.370	1.315	4.0	
			443	1.323	1.269	4.1	
			463	1.288	1.223	5.1	
Si(OC_6H_{13})$_4$	630.2	*779.1*	303	1.582	1.696	7.2	2
			323	1.569	1.651	5.2	
			343	1.544	1.607	4.1	
			363	1.497	1.564	4.4	
			383	1.468	1.521	3.6	
			403	1.427	1.479	3.6	
			423	1.384	1.437	3.8	
			443	1.345	1.395	3.7	
			463	1.306	1.353	3.6	
Si[$OCH_2C(C_2H_5)HC_2H_5$]$_4$	605.2	*743.8*	303	1.574	1.597	1.5	2
			323	1.564	1.552	0.7	
			343	1.539	1.509	2.0	
			363	1.494	1.466	1.9	
			383	1.466	1.423	2.9	
			403	1.427	1.381	3.2	
			423	1.381	1.339	3.1	
			443	1.340	1.296	3.3	
			463	1.297	1.254	3.3	
Si(OC_7H_{15})$_4$	670.7	*851.0*	303	1.596	1.754	9.9	2
			323	1.571	1.711	8.9	
			343	1.545	1.669	8.1	
			363	1.504	1.629	8.3	
			383	1.471	1.589	8.0	
			403	1.430	1.549	8.4	
			423	1.382	1.511	9.3	
			443	1.343	1.427	9.6	
			463	1.326	1.433	8.1	
Si(OC_8H_{17})$_4$	689.7	*914.1*	303	1.628	1.743	7.0	2
			323	1.604	1.703	6.1	
			343	1.572	1.664	5.8	
			363	1.546	1.626	5.8	
			383	1.504	1.589	5.6	
			403	1.470	1.553	5.6	
			423	1.432	1.517	5.9	
			443	1.376	1.482	7.7	
			463	1.358	1.447	6.5	
Si[$OCH_2C(C_2H_5)HC_4H_9$]$_4$	639.7	*831.3*	303	1.616	1.562	3.4	2
			323	1.598	1.523	4.7	

Table A.11. (Continued)

compound	T_b/K	T_c/K	T/K	exptl $k/(10^{-1}$ W m^{-1} K$^{-1})$	pred $k/(10^{-1}$ W m^{-1} K$^{-1})$	% dev	ref
$Si[OCH_2C(C_2H_5)HC_4H_9]_4$	639.7	*831.3*	343	1.569	1.485	5.4	
			363	1.529	1.448	5.3	
			383	1.492	1.411	5.4	
			403	1.458	1.375	5.7	
			423	1.410	1.340	5.0	
			443	1.367	1.304	4.6	
			463	1.352	1.269	6.2	
$Si(OC_{10}H_{21})_4$	758.2	*1168.4*	303	1.660	1.848	11.3	2
			323	1.628	1.813	11.3	
			343	1.607	1.778	10.7	
			363	1.589	1.745	9.8	
			383	1.564	1.713	9.5	
			403	1.534	1.682	9.7	
			423	1.478	1.652	11.8	
			443	1.436	1.622	13.0	
			463	1.409	1.594	13.1	
$Si(OC_{12}H_{25})_4$	809.2	*1644.4*	303	1.682	1.916	13.9	2
			323	1.647	1.885	14.4	
			343	1.621	1.855	14.4	
			363	1.593	1.827	14.7	
			383	1.570	1.800	14.7	
			403	1.539	1.774	15.3	
			423	1.494	1.749	17.1	
			443	1.447	1.725	19.2	
			463	1.424	1.701	19.5	
$C_2H_3Si(OC_2H_5)_3$	476.5	*576.7*	305	1.55	1.65	6.7	91
$C_2H_5Si(OC_2H_5)_3$	432.1	*573.1*	305	1.55	1.46	5.8	91
$(CH_3)_3SiCl$	333.2	497.8	305	1.26	1.33	5.6	91
$(CH_3)_2SiCl_2$	343.5	520.4	305	1.30	1.27	2.3	91
$H(CH_3)SiCl_2$	315.1	*483.2*	305	1.21	1.26	3.9	91
CH_3SiCl_3	338.8	517.4	305	1.42	1.17	17.3	91
$C_2H_5SiCl_3$	371.6	560.0	305	1.26	1.20	4.8	91
$C_3H_7SiCl_3$	359.9	*577.2*	305	1.21	1.18	2.6	91
$C_4H_9SiCl_3$	422.1	*603.6*	304	1.13	1.17	4.0	91
$C_5H_{11}SiCl_3$	444.2	*623.3*	304	1.13	1.16	2.6	91
$C_9H_{19}SiCl_3$	506.1	*667.7*	304	1.05	1.08	2.5	91
$(C_2H_5)_2SiCl_2$	403.6	595.8	305	1.34	1.28	4.3	91
$(C_5H_{11})_2SiCl_2$	556.3	*732.6*	304	1.00	1.19	18.3	91
$H(C_2H_5)SiCl_2$	314.1	*470.2*	305	1.21	1.15	4.6	91
$CH_2{=}CHCH_2SiCl_3$	381.1	*558.5*	305	1.21	1.15	4.8	91
$(C_2H_5)(C_2H_3)SiCl_2$	429.3	*579.8*	305	1.30	1.27	2.7	91
$C_2H_3SiCl_3$	363.8	*545.2*	305	1.30	1.18	9.1	91
$C_6H_5SiCl_3$	474.1	*687.5*	305	1.26	1.22	3.3	91
$(C_6H_5)_2SiCl_2$	577.0	*798.3*	304	1.13	1.22	8.0	91
$C_6H_{11}SiCl_3$	481.2	*690.1*	304	1.09	1.21	10.7	91
			Compound Basis				
av % dev						6.7	
% bias						0.3	
			Data Point Basis				
av % dev						7.1	
% bias						0.6	

[a] Deviations are absolute. Critical temperatures predicted by the Lyderson method are italic.

Table A.12. Predictions of Parachors for Organometallics[a]

compound	pts	temp range T_{low}	T_{high}	exptl parachor	% dev	pred parachor	% dev	ref
$Si(CH_3)_4$	1	293.2	293.2	261.1	-	252.3	12.8	119
$Si(C_2H_5)_4$	8	285.2	398.7	411.6	1.5	412.3	1.1	119, 176
$Si(C_3H_7)_4$	4	287.2	358.7	565.0	0.5	572.3	5.3	176
$Si(C_6H_5)_4$	4	518.2	552.2	787.4	0.2	788.7	0.7	176
$(C_2H_5)_3SiH$	2	293.2	298.2	339.4	0.3	332.3	8.1	110
$(CH_3)_3SiC_6H_5$	7	293.2	323.2	388.6	1.8	386.4	2.4	3, 118
$(CH_3)_2Si(C_6H_5)_2$	7	293.2	323.2	516.5	1.8	520.5	3.2	3, 118
$Si(OCH_3)_4$	4	291.2	334.2	330.6	2.0	331.5	2.2	176
$Si(OC_2H_5)_4$	6	289.7	333.7	485.3	2.3	491.5	5.3	119, 176
$Si(OC_3H_7)_4$	2	293.2	303.0	632.3	0.1	648.9	8.8	119
$(CH_3)_2Si(OC_3H_7)_2$	5	288.2	328.2	453.4	0.5	451.9	1.3	105
$(CH_3)_2Si(OC_4H_9)_2$	5	288.2	328.2	532.3	0.8	531.9	0.8	105
$C_2H_5Si(OC_2H_5)_3$	5	288.2	328.2	464.6	0.3	471.7	6.2	105
$C_2H_5Si(OC_3H_7)_3$	5	288.2	328.2	586.2	0.7	591.7	3.8	105
$C_2H_5Si(OC_4H_9)_3$	5	288.2	328.2	703.3	0.7	711.7	4.9	105
$(C_2H_5)_2Si(OC_3H_7)_2$	5	288.2	328.2	527.3	0.6	531.9	3.5	105
$(C_2H_5)_2Si(OC_4H_9)_2$	5	288.2	328.2	605.5	0.7	611.9	4.3	105
$C_6H_5Si(OC_2H_5)_3$	5	288.2	328.2	558.3	0.7	565.8	5.5	105

Table A.12. (Continued)

compound	pts	temp range		exptl parachor	% dev	pred parachor	% dev	ref
		T_{low}	T_{high}					
$(C_6H_5)Si(OC_4H_9)_3$	5	288.2	328.2	792.1	0.7	805.8	7.1	105
$(C_6H_5)Si(OC_2H_5)_2$	5	288.2	328.2	633.0	0.7	640.1	4.5	105
$(C_6H_5)_2Si(OC_3H_7)_2$	5	288.2	328.2	710.6	0.7	720.0	5.4	105
$(C_6H_5)_2Si(OC_4H_9)_2$	5	288.2	328.2	790.7	0.7	800.1	4.8	105
$(C_6H_5)C_3H_6Si(OC_2H_5)_3$	8	293.2	363.2	692.2	0.2	705.6	8.0	44
$HSi(OC_2H_5)_3$	1	298.2	298.2	388.9	-	391.7	2.9	110
$(CH_3)_3SiOH$	1	293.2	293.2	229.5	-	226.6	5.0	147
CH_3SiCl_3	8	293.2	363.2	249.2	1.1	251.4	7.2	147, 165
$(CH_3)_2SiCl_2$	1	293.2	293.2	256.1	-	251.7	6.7	147
$(CH_3)_3SiCl$	3	293.2	314.2	259.0	2.4	252.0	10.3	119, 147
$C_2H_5SiHCl_2$	2	293.2	298.2	254.7	0.4	251.7	4.6	110
$(C_2H_5)_2SiHCl$	2	293.2	298.2	299.7	0.0	292.0	9.9	110
$Si(OC_2H_4Cl)_4$	1	293.2	293.2	648.1	-	650.3	1.4	92
$Si[OCH(CH_2Cl)_2]_4$	1	293.2	293.2	947.1	-	954.3	3.1	92
$(CH_3)_3SiBr$	3	298.2	318.2	273.4	0.4	264.8	12.0	118
$(CH_3)_2SiBr_2$	3	298.2	318.2	282.9	0.5	277.3	7.7	118
$(CH_3)_2(C_6H_5)SiBr$	3	298.2	318.2	392.7	0.6	398.9	6.5	118
$(CH_3)(C_2H_5)_2SiBr$	3	298.2	318.2	347.0	0.3	344.8	2.5	118
$[C_6H_{13}(CH_3)_2Si]_2NH$	7	293.2	353.2	813.6	0.4	799.8	6.5	103
$[C_7H_{15}(CH_3)_2Si]_2NH$	7	293.2	353.2	893.5	0.4	879.8	5.9	103
$[C_8H_{17}(CH_3)_2Si]_2NH$	7	293.2	353.2	968.9	0.2	959.8	3.6	103
$[(CH_3)_3Si]_2NH$	13	298.2	368.2	437.2	1.4	423.6	11.8	74, 127
$(C_2H_5O)_2(CH_3)Si(CH_2)_2CN$	7	293.2	353.2	457.3	1.6	463.5	5.6	102
$(C_4H_9O)_2(CH_3)Si(CH_2)_2CN$	7	293.2	353.2	615.3	1.2	623.5	5.5	102
$(C_6H_{13}O)_2(CH_3)Si(CH_2)_2CN$	7	293.2	353.2	776.4	1.1	783.5	3.7	102
$(C_8H_{17}O)_2(CH_3)Si(CH_2)_2CN$	7	293.2	353.2	938.1	1.0	943.5	2.3	102
$(C_{10}H_{21}O)_2(CH_3)Si(CH_2)_2CN$	6	298.2	348.2	1096.2	1.0	1103.5	2.7	102
$(C_4H_9O)_3Si(CH_2)_2CN$	6	298.2	348.2	742.2	0.4	763.3	11.9	101
$(C_6H_{13}O)_3Si(CH_2)_2CN$	6	298.2	348.2	980.2	0.7	1003.3	9.8	101
$(C_8H_{17}O)_3Si(CH_2)_2CN$	6	298.2	348.2	1220.9	1.0	1243.3	7.6	101
$(C_{10}H_{21}O)_3Si(CH_2)_2CN$	6	298.2	348.2	1454.6	1.4	1483.3	8.1	101
Si_3H_8	1	293.2	293.2	259.8	-	254.3	8.3	54
Si_4H_{10}	1	293.2	293.2	329.3	-	328.7	0.7	54
$HSi(SiH_3)_3$	1	293.2	293.2	323.2	-	325.0	2.3	54
$HSi(SiH_3)_2(Si_2H_5)$	1	293.2	293.2	398.7	-	399.5	0.7	54
Si_5H_{12}	1	293.2	293.2	401.3	-	403.2	1.9	54
$HSi(SiH_3)_2(Si_3H_7)$	1	293.2	293.2	475.2	-	473.9	1.1	54
Si_6H_{14}	1	293.2	293.2	474.3	-	477.6	2.8	54
Si_7H_{16}	1	293.2	293.2	549.4	-	552.0	2.0	54
$SiCl_4$	8	296.2	328.2	240.2	1.3	251.1	19.4	134
$SiHCl_3$	18	273.2	313.2	207.5	0.6	211.4	7.8	110, 134
SiH_2I_2	1	288.3	288.3	266.4	-	241.9	32.1	47
SiH_3I	1	288.2	288.2	182.0	-	167.1	29.0	47
MM	22	272.1	358.2	422.3	1.8	413.4	8.2	3, 63, 68, 85, 119, 192
MDM	4	273.2	303.2	582.8	2.5	574.5	5.5	63, 68, 85, 192
MD_2M	4	273.2	303.2	743.5	2.3	735.6	4.2	63, 68, 85, 105, 192
D_3M	4	273.2	303.2	907.9	2.3	896.7	4.8	63, 68, 85, 192
MD_4M	3	273.2	298.2	1068.6	2.3	1057.7	4.0	63, 85, 192
MD_5M	3	273.2	298.2	1229.0	2.8	1218.8	3.7	63, 85, 192
MD_6M	3	273.2	298.2	1392.5	2.3	1379.9	3.5	63, 85, 192
MD_7M	2	273.2	273.2	1559.6	0.9	1541.0	4.7	63, 192
$MD_{10}M$	1	273.2	273.2	2041.1	-	2024.3	3.3	63
$MD_{15}M$	2	273.2	308.2	2831.9	0.6	2829.7	0.6	63
D_4	10	273.2	313.2	645.7	1.3	651.4	3.6	84, 119, 127, 192
D_5	4	273.2	301.7	802.0	1.9	808.5	3.3	84, 119, 192
D_6	2	273.2	298.2	958.8	4.4	967.3	4.6	84, 192
D_7	2	273.2	298.2	1118.4	2.6	1127.6	3.4	84, 192
M“M”	6	333.2	383.2	958.9	1.2	949.8	3.8	108
M“D’M	6	333.2	383.2	1001.7	2.4	976.8	9.5	108
M“’D’M	6	333.2	383.2	1117.3	3.1	1110.9	3.4	108
M“D’M’	6	333.2	383.2	1138.5	2.6	1110.9	9.3	108
M“’D’M’	6	333.2	383.2	1267.6	3.0	1245.0	6.9	108
M“D’M”	6	333.2	383.2	1223.9	0.9	1245.0	7.1	108
M“D’$_2$M”	6	333.2	383.2	1494.9	1.2	1449.6	11.6	108
$[(C_2H_5)_3Si]_2O$	1	303.2	303.2	631.5	-	653.4	14.6	68
$Si_4(C_2H_5)_{10}O_3$	1	303.2	303.2	1104.6	-	1135.6	11.7	68
$Si_5(C_2H_5)_{12}O_4$	1	303.2	303.2	1334.7	-	1376.7	13.2	68
$[C_6H_{13}(CH_3)_2Si]_2O$	7	273.2	353.2	811.5	0.1	813.4	0.9	103
$[C_7H_{15}(CH_3)_2Si]_2O$	7	273.2	353.2	897.3	0.4	893.4	1.8	103
$[C_8H_{17}(CH_3)_2Si]_2O$	7	273.2	353.2	966.2	0.2	973.4	3.0	103
$[C_9H_{19}(CH_3)_2Si]_2O$	7	273.2	353.2	1039.9	0.7	1053.4	5.3	103
$[C_7H_{15}(CH_3)_2SiOSi(CH_3)_2]_2O$	7	273.2	353.2	1217.2	0.5	1215.6	0.7	103
$[C_9H_{19}(CH_3)_2SiOSi(CH_3)_2]_2O$	7	273.2	353.2	1367.9	0.3	1375.6	2.3	103
FD_3	7	273.2	353.2	750.0	0.7	762.2	6.6	104
F_2D_2	7	273.2	353.2	860.3	0.3	874.0	6.5	104

Table A.12. (Continued)

compound	pts	temp range T_{low}	temp range T_{high}	exptl parachor	% dev	pred parachor	% dev	ref
F_3D	7	273.2	353.2	971.2	0.4	985.8	6.1	104
F_3D_2	7	273.2	353.2	1114.8	1.0	1143.9	10.9	104
F_4D	7	273.2	353.2	1226.5	0.3	1255.7	9.9	104
$B(C_2H_5)_3$	8	273.2	323.2	306.9	0.7	299.7	9.0	100, 106
$B(C_4H_9)_3$	1	306.2	306.2	526.1	-	539.7	10.7	83
$B(i\text{-}C_5H_{11})_3$	1	306.2	306.2	659.3	-	648.8	6.1	83
$B(C_5H_{11})_3$	1	306.2	306.2	683.7	-	659.7	13.4	83
$B(C_6H_{13})_3$	1	306.2	306.2	795.6	-	779.7	7.8	83
$B(OCH_3)_3$	5	298.2	333.2	234.8	0.9	239.1	7.2	30, 50
$B(OC_2H_5)_3$	8	298.2	363.2	355.9	1.3	359.1	3.8	30, 50
$B(OC_3H_7)_3$	11	298.2	403.2	474.3	1.3	479.1	4.1	30
$B(O\text{-}iC_3H_7)_3$	10	298.2	403.2	471.0	2.6	472.5	2.8	30
$B(OC_4H_9)_3$	11	298.2	423.2	595.9	2.0	599.1	2.7	30
$B(O\text{-}iC_4H_9)_3$	11	298.2	423.2	589.4	0.8	592.5	2.1	30
$(CH_3)_2NBCl_2$	14	233.2	298.2	251.4	1.0	252.1	1.4	24
$(C_2H_5)_2NBCl_2$	11	283.2	333.2	331.9	1.1	332.1	1.1	138
$B(OC_2H_4Cl)_3$	1	273.2	273.2	488.1	-	478.2	7.9	92
$B[OCH(CH_2Cl)_2]_3$	1	273.2	273.2	722.2	-	706.2	8.6	92
$(C_4H_9BO)_3$	9	273.6	303.3	640.2	0.7	640.2	0.7	113
$BF_3(C_2H_5)_2O$	4	218.2	248.2	305.4	0.6	302.3	4.0	195
B_2H_6	6	165.0	302.7	121.9	0.6	119.4	1.1	100, 163
BF_3	5	153.2	173.2	87.1	0.3	91.5	21.6	195
BBr_3	10	295.2	357.2	220.5	0.8	217.2	6.1	89, 100
$Al(CH_3)_3$	7	273.2	413.2	208.4	0.5	201.4	9.2	204
$Al(C_2H_5)_3$	7	273.2	413.2	314.5	0.3	321.4	11.1	204
$Al(C_3H_7)_3$	7	273.2	413.2	429.4	0.6	441.4	12.9	204
av % dev					1.1		6.1	
% bias							0.3	

[a] All T are in kelvin, parachors are in $mN^{1/4}\ m^{11/4}\ kmol^{-1}$, and deviations are absolute. Molecular abbreviations: $M = (CH_3)_3SiO_{0.5}$, $M' = (C_6H_5)(CH_3)_2SiO_{0.5}$, $D = (CH_3)_2SiO$, $F = (CH_3)(CF_3CH_2CH_2)SiO$, $M'' = (CH_3)(C_6H_5)_2SiO_{0.5}$, $M''' = (C_6H_5)_3SiO_{0.5}$, $D' = (CH_3)(C_6H_5)SiO$

Data References

(1) Adame, I. E.; Vicharelli, P. A. *Bull. Soc. Chim. Belg.* **1978**, *87*, 339.
(2) Alagar, M.; Krishnasamy, V. *Hung. J. Ind. Chem.* **1987**, *15*, 453.
(3) Aleksandrova, Z. A.; Gundyrev, A. A.; Nametkin, N. S.; Panchenkov, G. M.; Topchiev, A. V. *Issled. Obl. Kremniiorg. Akad. Nauk SSSR* **1962**, 219.
(4) Ambrose, D. NPL Report Chem. 107; National Physical Laboratory: Middlesex, U.K., February 1980.
(5) Ambrose, D. Supplement to NPL Report Chem. 107; National Physical Laboratory: Middlesex, U.K., June 1987.
(6) Bains, S. K.; Noble, P. N.; Walsh, R. *J. Chem. Soc., Faraday Trans. 2* **1986**, *82*, 837.
(7) Baldwin, J. C.; Lappert, M. F.; Pedley, J. B.; Poland, J. S. *J. Chem. Soc., Dalton Trans.* **1972**, 1943.
(8) Baldwin, J. C.; Lappert, M. F.; Pedley, J. B.; Treverton, J. A. *J. Chem. Soc. A* **1967**, 1980.
(9) Bamford, C. H.; Levi, D. L.; Newitt, D. M. *J. Chem. Soc.* **1946** 468.
(10) Beezer, A. E.; Mortimer, C. T. *J. Chem. Soc. A* **1966**, 514.
(11) Bennett, F.; Lielmezs, J. *Thermochim. Acta* **1981**, *44*, 43.
(12) Bennett, J. E.; Skinner, H. A. *J. Chem. Soc.* **1962**, 2150.
(13) Benson, S. W.; Cruickshank, F. R.; Golden, D. M.; Haugen, G. R.; O'Neal, H. E.; Rodgers, A. S.; Shaw, R.; Walsh, R. *Chem. Rev.* **1969**, *69*, 279.
(14) Birr, K. H. *Z. Anorg. Allg. Chem.* **1962**, *315*, 175.
(15) Booth, H. S.; Carnell, P. H. *J. Am. Chem. Soc.* **1946**, *68*, 2650.
(16) Booth, H. S.; Halbedel, H. S. *J. Am. Chem. Soc.* **1946**, *68*, 2652.
(17) Booth, H. S.; Jarry, R. L. *J. Am. Chem. Soc.* **1949**, *71*, 971.
(18) Booth, H. S.; Martin, W. F. *J. Am. Chem. Soc.* **1946**, *68*, 155.
(19) Booth, H. S.; Schwartz, A. A. *J. Am. Chem. Soc.* **1946**, *68*, 2662.
(20) Booth, H. S.; Spessard, D. R. *J. Am. Chem. Soc.* **1946**, *68*, 2660.
(21) Booth, H. S.; Suttle, J. F. *J. Am. Chem. Soc.* **1946**, *68*, 2658.
(22) Brotherton, R. J.; McCloskey, A. L.; Boone, J. L.; Manasevit, H. M. *J. Am. Chem. Soc.* **1960**, *82*, 6245.
(23) Brotherton, R. J.; McCloskey, A. L.; Petterson, L. L.; Steinberg, H. *J. Am. Chem. Soc.* **1960**, *82*, 6242.
(24) Brown, C. A.; Osthoff, R. C. *J. Am. Chem. Soc.* **1952**, *74*, 2340.
(25) Burg, A. B. *J. Am. Chem. Soc.* **1940**, *62*, 2228.
(26) Burg, A. B.; Banus, J. *J. Am. Chem. Soc.* **1954**, *76*, 3903.
(27) Burg, A. B.; Randolph, C. L. *J. Am. Chem. Soc.* **1951**, *73*, 953.
(28) Chai, B. J.; Ko, H. C.; Greenbaum, M. A.; Farber, M. *J. Phys. Chem.* **1967**, *71*, 3331.
(29) Chase, M. W., Jr.; Davies, C. A.; Downey, J. R., Jr.; Frurip, D. J.; McDonald, R. A.; Syverud, A. N. JANAF Thermochemical Tables. *J. Phys. Chem. Ref. Data* **1985**, *14* (Suppl. 1).
(30) Christopher, P. M.; Guerra, G. V. *J. Chem. Eng. Data* **1971**, *16*, 468.
(31) Christopher, P. M.; Shilman, A. *J. Chem. Eng. Data* **1967**, *12*, 333.
(32) Claydon, A. P.; Mortimer, C. T. *J. Chem. Soc.* **1962**, 3212.
(33) Coates, G. E. *J. Chem. Soc.* **1950**, 3481.
(34) Cooper, W. J.; Masi, J. F. *J. Phys. Chem.* **1960**, *64*, 682.
(35) Cox, J. D.; Pilcher, J. *Thermochemistry of Organic and Organometallic Compounds*; Academic Press: London, 1970.
(36) Cox, J. D.; Wagman, D. D.; Medvedev, V. A. *CODATA Key Values for Thermodynamics*; Hemisphere Publishing Corp.: New York, 1989.
(37) Cyvin, S. J.; Cyvin, B. N.; Rao, D. B.; Snelson, A. *Z. Anorg. Allg. Chem.* **1971**, *380*, 212.
(38) Cyvin, J.; Torset, O. *Rev. Chim. Miner.* **1972**, *9*, 179.
(39) Da Silva, V. A. V.; Reis, A. M. V. *Rev. Port. Quim.* **1978**, *20*, 47.
(40) Dhanalakshmi, A.; Kamala, P. *Acta Cien. Indica* **1983**, *9*, 1.
(41) Dhanalakshmi, A.; Kamala, P.; Lalitha, M. *Indian J. Pure Appl. Phys.* **1982**, *20*, 830.
(42) Dickinson, E.; McLure, I. A. *J. Chem. Soc., Faraday Trans. 2* **1974**, *70*, 2313.
(43) Ditsent, V. E.; Skorokhodov, I. I.; Terent'eva, N. A.; Zolotareva, M. N. *Russ. J. Phys. Chem.* **1972**, *46*, 1088.
(44) Ditsent, V. E.; Skorokhodov, I. I.; Terent'eva, N. A.; Zolotareva, M. N.; Lavygin, I. A.; Pritbytko, A. M.; Zaitseva, L. Ya.; Pomerantseva, M. G.; Belyakova, Z. V. *Russ. J. Phys. Chem.* **1977**, *51*, 599.
(45) Doncaster, A. M.; Walsh, R. *J. Chem. Soc., Faraday Trans. 2* **1986**, *82*, 707.
(46) Ebsworth, E. A. V.; Emeleus, H. J. *J. Chem. Soc.* **1958**, 2150.
(47) Emeleus, H. J.; Maddock, A. G.; Reid, C. *J. Chem. Soc.* **1941**, 353.
(48) Emeleus, H. J.; Wilkins, C. J. *J. Chem. Soc.* **1944**, 454.
(49) Ethyl Corp. Private communication, 1987.
(50) Etridge, J. J.; Sugden, S. *J. Chem. Soc.* **1928**, 989.
(51) Farber, M.; Srivastava, R. D. *Chem. Phys. Lett.* **1977**, *51*, 307.
(52) Farber, M.; Srivastava, R. D. *Chem. Phys. Lett.* **1979**, *60*, 216.
(53) Farber, M.; Srivastava, R. D. *J. Chem. Thermodyn.* **1979**, *11*, 939.
(54) Feher, F.; Hadicke, P.; Frings, H. *Inorg. Nucl. Chem. Lett.* **1973**, *9*, 931.
(55) Feher, F.; Jansen, G.; Rohmer, H. *Z. Anorg. Allg. Chem.* **1964**, *329*, 31.
(56) Fenwick, J. T. F.; Wilson, J. W. *J. Chem. Soc., Dalton Trans.* **1972**, 1324.
(57) Finch, A.; Gardner, P. J. *Prog. Boron Chem.* **1969**, *3*, 177.
(58) Finch, A.; Gardner, P. J.; Hill, N.; Hussian, K. S. *J. Chem. Soc., Dalton Trans.* **1973**, 2543.
(59) Finch, A.; Gardner, P. J.; Pearn, E. J.; Watts, G. B. *Trans. Faraday Soc.* **1967**, *63*, 1603.
(60) Finch, A.; Gardner, P. J.; Pearn, E. J.; Watts, G. B. *Trans. Faraday Soc.* **1967**, *63*, 1880.
(61) Flaningam, O. L. *J. Chem. Eng. Data* **1986**, *31*, 266.
(62) Flitcroft, T.; Skinner, H. A. *J. Chem. Soc.* **1956**, 3355.

(63) Fox, H. W.; Taylor, P. W.; Zisman, W. A. *Ind. Eng. Chem.* **1947**, *39*, 1401.
(64) Gadzhiev, S. N.; Agarunov, M. Y. *Russ. J. Phys. Chem.* **1965**, *39*, 130.
(65) Gal'chenko, G. L.; Brykina, E. P.; Varushchenko, R. M.; Vasil'ev, L. S.; Mikhailov, B. M. *Russ. J. Phys. Chem.* **1973**, *47*, 914.
(66) Glushko, V. P. Thermal Constants of the Substances; Academy of Sciences: Moscow, USSR, 1970; Vol. 4, Part 1.
(67) Goldblum, K. B.; Moody, L. S. *Ind. Eng. Chem.* **1955**, *47*, 847.
(68) Golik, O. Z.; Cholpan, P. P. *Ukr. Fiz. Zh.* (*Ukr. Ed.*) **1960**, *5*, 242.
(69) Golosova, R. M.; Arkhipova, S. F.; Mosin, A. M.; Karapet'yants, M. K. *Russ. J. Phys. Chem.* **1967**, *41*, 781.
(70) Golosova, R. M.; Korobov, V. V.; Karapet'yants, M. K. *Russ. J. Phys. Chem.* **1971**, *45*, 598.
(71) Golosova, R. M.; Korobov, V. V.; Karapet'yants, M. K. *Russ. J. Phys. Chem.* **1971**, *45*, 765.
(72) Golosova, R. M.; Mosin, A. M.; Karapet'yants, M. K. *Russ. J. Phys. Chem.* **1967**, *41*, 780.
(73) Good, W. D.; Lacina, J. L.; DePrater, B. L.; McCullough, J. P. *J. Phys. Chem.* **1964**, *68*, 579.
(74) Grinberg, E. E.; Chernaya, N. G.; Bershitskii, A. M.; Nechaeva, G. Yu.; Abuzin, Yu. M.; Efremov, A. A. *Russ. J. Phys. Chem.* **1986**, *60*, 779.
(75) Guest, M. F.; Pedley, J. B.; Horn, M. *J. Chem. Thermodyn.* **1969**, *1*, 345.
(76) Gunn, S. R.; Green, L. G. *J. Phys. Chem.* **1961**, *65*, 178.
(77) Gunn, S. R.; Green, L. G. *J. Phys. Chem.* **1961**, *65*, 779.
(78) Gunn, S. R.; Green, L. G. *J. Phys. Chem.* **1964**, *68*, 946.
(79) Hajiev, S. N.; Agarunov, M. J. *J. Organomet. Chem.* **1968**, *11*, 415.
(80) Hay, J. N.; Hooper, P. G.; Robb, J. C. *Trans. Faraday Soc.* **1969**, 1365.
(81) Hicks, C. P.; Young, C. L. *J. Chem. Soc., Faraday Trans.* **1971**, *67*, 1598.
(82) Hicks, C. P.; Young, C. L. *J. Chem. Soc., Faraday Trans. 1* **1976**, *72*, 122.
(83) Hughes, R. L.; Smith, I. C.; Lawless, E. W. *Production of the Boranes and Related Research*; Academic Press: New York, 1967.
(84) Hunter, M. J.; Hyde, J. H.; Warrick, E. L.; Fletcher, H. J. *J. Am. Chem. Soc.* **1946**, *68*, 667.
(85) Hunter, M. J.; Warrick, E. L.; Hyde, J. F.; Currie, C. C. *J. Am. Chem. Soc.* **1946**, *68*, 2284.
(86) Iseard, B. S.; Pedely, J. B.; Traverton, J. A. *J. Chem. Soc. A* **1971**, 3095.
(87) Ivannikov, P. S.; Litvinenko, I. V.; Radchenko, I. V. *J. Eng. Phys.* **1975**, *28*, 63.
(88) Jakes, J.; Papousek, D. *Collect. Czech. Chem. Commun.* **1961**, *26*, 2110.
(89) Jasper, J. J. *J. Phys. Chem. Ref. Data* **1972**, *1*, 843.
(90) Jenkins, A. C.; Chambers, G. F. *Ind. Eng. Chem.* **1954**, *46*, 2367.
(91) Jenkins, A. C.; Reid, A. J. *Ind. Eng. Chem.* **1954**, *46*, 2566.
(92) Jones, W. J.; Thomas, L. H.; Pritchard, E. H.; Bowden, S. T. *J. Chem. Soc.* **1946**, 824.
(93) Klyuchnikov, V. A.; Danilova, T. F.; Voronkov, M. G.; D'yakov, V. M. *Dokl. Akad. Nauk SSSR* **1985**, *281*, 373.
(94) Kol'yakova, G. M.; Rabinovich, I. B.; Vyazankin, N. S. *Dokl. Akad. Nauk SSSR* **1971**, *200*, 111.
(95) Kol'yakova, G. M.; Rabinovich, I. B.; Vyazankin, N. S. *Dokl. Akad. Nauk SSSR* **1971**, *200*, 735.
(96) Krasavin, A. M.; Golosova, R. M.; Shlyakova, V. G. *Russ. J. Phys. Chem.* **1977**, *51*, 5.
(97) Krishna Pillai, M. G.; Ramaswamy, A. *Acta Phys. Pol.* **1964**, *25*, 627.
(98) Kvande, H. *High Temp.—High Pressures* **1983**, *15*, 677.
(99) Lapidus, I. I.; Nisel'son, C. A.; Seifer, A. L. *Thermophysical Properties of Gases and Liquids*; Rabinovitz, V. A, ed.; Translated from Russian, published for U.S. Department of Commence and NSF by Israel Program for Scientific Translations: Jerusalem, 1970; No. 1, p 102.
(100) Laubengayer, A. W.; Ferguson, R. P.; Newkirk, A. E. *J. Chem. Soc.* **1941**, *63*, 559.
(101) Lavygin, I. A.; Gol'din, G. S.; Smirnova, E. S.; Bespolova, Yu. I.; Chalbysheva, N. V. *Zh. Prikl. Khim.* **1984**, *57*, 1365.
(102) Lavygin, I. A.; Gol'din, G. S.; Smirnova, E. S.; Bespolova, Yu. I.; Poddubnyi, V. G. *Zh. Prikl. Khim.* **1983**, *56*, 337.
(103) Lavygin, I. A.; Izmailov, B. A.; Zhdanov, A. A.; Myakushev, V. D.; Skorokhodov, I. I.; Migalina, V. M. *Zh. Prikl. Khim.* **1980**, *53*, 1155.
(104) Lavygin, I. A.; Skorokhodov, I. I.; Kleinovskaya, M. A.; Potashova, G. A.; Yur'eva, A. M. *Russ. J. Phys. Chem.* **1978**, *52*, 893.
(105) Lavygin, I. A.; Skorokhodov, I. I.; Leitan, O. V.; Balukov, Yu. L.; Dubinina, K. M. *Inorg. Mater.* **1982**, *18*, 696.
(106) Lavygin, I. A.; Skorokhodov, I. I.; Shmyreva, G. O.; Zhigach, A. F.; Petrunin, A. B.; Krasavin, A. M.; Golosova, R. M.; Shlyakova, V. G. *Russ. J. Phys. Chem.* **1977**, *51*, 5.
(107) Lavygin, I. A.; Skorokhodov, I. I.; Shmyreva, G. O.; Zhigach, A. F.; Petrunin, A. B.; Krasavin, A. M.; Golosova, R. M.; Shlyakova, V. G. *Russ. J. Phys. Chem.* **1977**, *51*, 1270.
(108) Lavygin, I. A.; Skorokhodov, I. I.; Zaitseva, L. Ya.; Potashova, G. A.; Kleinovskaya, M. A.; Blekh, L. M. *Inorg. Mater.* **1978**, *14*, 596.
(109) Lesiecki, M. L.; Shirk, J. S. *J. Chem. Phys.* **1972**, *56*, 4171.
(110) MacKenzie, C. A.; Mills, A. P.; Scott, J. M. *J. Am. Chem. Soc.* **1950**, *72*, 2032.
(111) Mann, D. E. *J. Chem. Phys.* **1954**, *22*, 762.
(112) Mathews, J. F. *Chem. Rev.* **1972**, *72*, 71.
(113) Mattraw, H. C.; Erickson, C. E.; Laubengayer, A. W. *J. Am. Chem. Soc.* **1956**, *78*, 4901.
(114) McGlashan, M. L.; McKinnon, I. R. *J. Chem. Thermodyn.* **1977**, *9*, 1205.
(115) McLure, I. A.; Neville, J. F. *J. Chem. Thermodyn.* **1977**, *9*, 957.
(116) McLure, I. A.; Neville, J. F. *J. Chem. Thermodyn.* **1982**, *14*, 385.
(117) Mikawa, Y. *J. Chem. Soc. Jpn.* **1960**, *81*, 1512.
(118) Mills, A. P.; Becker, W. E. *J. Phys. Chem.* **1956**, *60*, 1644.
(119) Mills, A. P.; MacKenzie, C. A. *J. Am. Chem. Soc.* **1954**, *76*, 2672.
(120) Mortimer, C. T.; Sellers, P. W. *J. Chem. Soc.* **1963**, 1978.
(121) Mosin, A. M. *Russ. J. Phys. Chem.* **1975**, *49*, 437.
(122) Mosin, A. M.; Golosova, R. M. *Russ. J. Phys. Chem.* **1971**, *45*, 750.
(123) Mosin, A. M.; Mikhailov, A. M. *Russ. J. Phys. Chem.* **1972**, *46*, 313.
(124) Mosin, A. M.; Shaulov, Y. K. *Russ. J. Phys. Chem.* **1972**, *46*, 1051.
(125) Mosin, A. M.; Shavlov, Y. K. *Russ. J. Phys. Chem.* **1972**, *46*, 1055.
(126) Mosin, A. M.; Shaulov, Y. K.; Markova, I. Y.; Krylov, V. V. *Russ. J. Phys. Chem.* **1975**, *49*, 140.
(127) Myers, R. S.; Clever, H. L. *J. Chem. Eng. Data* **1969**, *14*, 161.
(128) Myers, J. E.; Hershey, H. C.; Kay, W. B. *J. Chem. Thermodyn.* **1979**, *11*, 1019.
(129) Nagarajan, G. *Bull. Soc. Chim. Belg.* **1962**, *71*, 65.
(130) Nagarajan, G. *Bull. Soc. Chim. Belg.* **1962**, *71*, 226.
(131) Nagarajan, G. *Bull. Soc. Chim. Belg.* **1964**, *73*, 811.
(132) Nagarajan, G. *Z. Phys. Chem.* **1962**, *31*, 347.
(133) Nagarajan, G. *Z. Phys. Chem.* **1963**, *223*, 27.
(134) Nisel'son, L. A.; Pugachevich, P. P.; Sokolova, T. D.; Bederdinov, R. A. *Russ. J. Inorg. Chem.* **1965**, *10*, 705.
(135) Nisel'son, L. A.; Sokolova, T. D.; Lapidus, I. I. *Russ. J. Inorg. Chem.* **1967**, *12*, 752.
(136) O'Neal, H. E.; Ring, M. A. *Inorg. Chem.* **1966**, *5*, 435.
(137) O'Neal, H. E.; Ring, M. A. *J. Organomet. Chem.* **1981**, *213*, 419.
(138) Osthoff, R. C.; Brown, C. A. *J. Am. Chem. Soc.* **1952**, *74*, 2378.
(139) Owenby, P. D.; Gretz, R. D. *Surf. Sci.* **1968**, *9*, 37.
(140) Parsons, T. D.; Silverman, M. B.; Ritter, D. M. *J. Am. Chem. Soc.* **1957**, *79*, 5091.
(141) Pedley, J. B.; Kirk, A.; Seilman, S.; Heath, L. G. *Computer Analysis of Thermochemical Data: Silicon Compounds*; University of Sussex: Sussex, 1972.
(142) Pedley, J. B.; Rylance, J. *Sussex-NPL. Computer Analyzed Thermochemical Data: Organic and Organometallic Compounds*; University of Sussex: Sussex, 1977.
(143) Pilcher, G.; Skinner, H. A. *The Chemistry of the Metal-Carbon Bond*; John Wiley & Sons: New York, 1982.
(144) Porter, R. F.; Gupta, S. K. *J. Phys. Chem.* **1964**, *68*, 2732.
(145) Rabinovich, I. B.; Kiparisova, E. G.; Aleksandrov, Y. A. *Dokl. Akad. Nauk SSSR* **1971**, *200*, 842.
(146) Reuther, H. *Chem. Tech.* (*Berlin*) **1950**, *2*, 331.
(147) Reuther, H. *Chem. Tech.* (*Berlin*) **1954**, *6*, 302.
(148) Ring, M. A.; O'Neal, H. E.; Kadhim, A. H.; Jappe, F. *J. Organomet. Chem.* **1966**, *5*, 124.
(149) Sathianandan, K.; Margrave, J. L. *J. Mol. Spectrosc.* **1963**, *10*, 442.
(150) Scott, D. W.; Messerly, J. F.; Todd, S. S.; Guthrie, G. B.; Hossenlopp, I. A.; Moore, R. T.; Osborn, A.; Berg, W. T.; McCullough, J. P. *J. Phys. Chem.* **1961**, *65*, 1320.
(151) Shanmugasundaram, G.; Nagarajan, G. *Z. Phys. Chem.* **1969**, *240*, 363.
(152) Shaulov, Y. K.; Shmyreva, G. O. *Russ. J. Phys. Chem.* **1968**, *42*, 1008.
(153) Shaulov, Y. K.; Shmyreva, G. O.; Tubyanskaya, V. S. *Russ. J. Phys. Chem.* **1965**, *39*, 51.
(154) Shaulov, Y. K.; Tubyanskaya, V. S.; Evstegneeva, E. V.; Shmyreva, G. O. *Russ. J. Phys. Chem.* **1964**, *38*, 967.
(155) Shinmei, M.; Imai, T.; Yokokawa, T.; Masson, C. R. *Proc. First Int. Symp. Molten Salts* **1983**, 133.
(156) Shmyreva, G. O.; Sakharovskaya, G. B.; Popov, A. F.; Korneev, I. N.; Smolyaninova, A. A. *Russ. J. Phys. Chem.* **1971**, *45*, 1970.
(157) Simmrock, K. H.; Janowsky, R.; Ohnsorge, A. *Critical Data of Pure Substances*; DECHEMA Chemistry Data Series; DECHEMA: Frankfurt, 1986; Vol. II.
(158) Sin'ko, S. V.; Pentin, Y. A.; Goldin, G. M.; Kuramshina, G. M. *Russ. J. Phys. Chem.* **1985**, *59*, 1604.
(159) Sin'ko, S. V.; Pentin, Y. A.; Goldin, G. M.; Kuramshina, G. M. *Russ. J. Phys. Chem.* **1985**, *59*, 1606.
(160) Skinner, H. A. *Adv. Organomet. Chem.* **1964**, *2*, 49.
(161) Skinner, H. A.; Smith, N. B. *J. Chem. Soc.* **1954**, 3930.
(162) Sladkov, I. B.; Rasina, M. I. *Russ. J. Phys. Chem.* **1982**, *56*, 631.
(163) Smith, S. H.; Miller, R. R. *J. Am. Chem. Soc.* **1950**, *72*, 1452.
(164) Sokolov, V. B.; Karapet'yants, M. K.; Rumyantseva, N. D.; Drozdov, V. A. *Russ. J. Phys. Chem.* **1971**, *45*, 1332.
(165) Sokolova, T. D.; Prokof'eva, N. K.; Nisel'son, L. A. *Russ. J. Phys. Chem.* **1973**, *47*, 154.
(166) Spangenberg, H. J. *Z. Phys. Chem.* **1966**, *232*, 271.
(167) Spangenberg, H. J.; Kriegsman, H. *Z. Phys. Chem.* **1963**, *224*, 273.
(168) Spangenberg, H. J.; Pfeiffer, M. *Z. Phys. Chem.* **1966**, *232*, 343.
(169) Steele, W. V. *J. Chem. Thermodyn.* **1978**, *10*, 445.
(170) Steele, W. V. *J. Chem. Thermodyn.* **1983**, *15*, 595.
(171) Stepanov, N. G. *Russ. J. Phys. Chem.* **1972**, *46*, 464.

(172) Stepanov, N. G.; Nozdrev, V. F. *Russ. J. Phys. Chem.* **1968**, *42*, 1300.
(173) Stock, A.; Somieski, C. *Ber. Dtsch. Chem. Ges.* **1919**, *52*, 695.
(174) Stull, D. R. *Ind. Eng. Chem.* **1947**, *39*, 517.
(175) Suga, H.; Seki, S. *Bull. Chem. Soc. Jpn.* **1959**, *32*, 1088.
(176) Sugden, S.; Wilkins, H. *J. Chem. Soc.* **1931**, 126.
(177) Takagi, S.; Ishikawa, M.; Kumada, M.; Kimura, T.; Fujishiro, R. *Thermochim. Acta* **1986**, *109*, 55.
(178) Tanaka, T. *Bull. Chem. Soc. Jpn.* **1959**, *32*, 1258.
(179) Tanaka, T.; Takahashi, U.; Okawara, R.; Watase, T. *J. Chem. Phys.* **1951**, *19*, 1330.
(180) Tanaka, T.; Watase, T. *J. Chem. Phys.* **1954**, *22*, 1268.
(181) Tannenbaum, S.; Kaye, S.; Lewenz, G. F. *J. Am. Chem. Soc.* **1953**, *75*, 3753.
(182) Tel'noi, V. I.; Rabinovich, I. B. *Russ. Chem. Rev.* **1980**, *49*, 603.
(183) Tel'noi, V. I.; Rabinovich, I. B. *Russ. J. Phys. Chem.* **1965**, *39*, 1239.
(184) Tel'noi, V. I.; Rabinovich, I. B. *Russ. J. Phys. Chem.* **1966**, *40*, 842.
(185) Urry, G.; Kerrigan, J.; Parsons, T. D.; Schlesinger, H. I. *J. Am. Chem. Soc.* **1954**, *76*, 5299.
(186) Urry, G.; Wartik, T.; Moore, R. E.; Schlesinger, H. I. *J. Am. Chem. Soc.* **1954**, *76*, 5293.
(187) Venkateswarlu, K.; Natarajan, A. *Acta Phys. Pol.* **1967**, *8*, 205.
(188) Voronkov, M. G.; Baryshok, V. P.; Klyuchnikov, V. A.; Danilova, T. F.; Pepekin, V. I.; Korchagina, A. N.; Khudobin, Y. I. *J. Organomet. Chem.* **1988**, *345*, 27.
(189) Voronkov, M. G.; Klyuchnikov, V. A.; Danilova, T. F.; Korchagina, A. N.; Baryshok, V. P.; Landa, L. M. *Izv. Akad. Nauk SSSR* **1986**, *9*, 1790.
(190) Voronkov, M. G.; Klyuchnikov, V. A.; Korchagina, A. N.; Danilova, T. F.; Shvets, G. N.; Baryshok, V. P.; D'yakov, V. M. *Izv. Akad. Nauk SSSR* **1986**, *9*, 1975.
(191) Wagman, D. D.; Evans, W. H.; Parker, V. B.; Schumm, R. H.; Halow, I.; Bailey, S. M.; Churney, K. L.; Nuttall, R. L. NBS Tables. *J. Phys. Chem. Ref. Data* **1982**, *11* (Suppl. 2).
(192) Waterman, H. I.; Van Herwijnen, W. E. R.; Den Hartog, H. W. *J. Appl. Chem.* **1958**, *8*, 625.
(193) Waterson, S. D.; Young, C. L. *Aust. J. Chem.* **1978**, *31*, 957.
(194) Webb, D. U.; Justice, B. H.; Prophet, H. *J. Chem. Thermodyn.* **1969**, *1*, 16.
(195) Wiberg, E.; Mathing, W. *Ber. Dtsch. Chem. Ges.* **1937**, *70B*, 690.
(196) Wiberg, E.; Ruschmann, W. *Ber. Dtsch. Chem. Ges.* **1937**, *70B*, 1393.
(197) Wiberg, V. E.; Schuster, K. *Z. Anorg. Allg. Chem.* **1933**, *213*, 77.
(198) Wiberg, V. E.; Sutterlin, W. *Z. Anorg. Allg. Chem.* **1931**, *202*, 1.
(199) Wilson, J. W.; Fenwick, J. T. F. *J. Chem. Thermodyn.* **1973**, *5*, 341.
(200) Wintgen, R. *Ber. Dtsch. Chem. Ges.* **1919**, *52*, 724.
(201) Young, C. L. *J. Chem. Soc., Faraday Trans. 1* **1972**, *68*, 580.
(202) Young, C. L. *J. Chem. Soc., Faraday Trans. 2* **1972**, *68*, 452.
(203) Young, C. L. *J. Chem. Thermodyn.* **1972**, *4*, 65.
(204) Zorin, A. D.; Kut'in, A. M.; Kuznetsova, T. V.; Klimov, K. N.; Feshchenko, I. A. *Russ. J. Phys. Chem.* **1984**, *58*, 1593.

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