

Calculation of Thermodynamic Properties in Pure Organic Compounds

Y.C. Li, C.P. Wang, and X.J. Liu

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The reduced Gibbs free energies of 30 types of pure organic compounds were calculated by using the Sanchez and Lacombe model (SL model). The calculated results for each pure organic compound are presented as both polynomial expressions and graphs. This database of pure organic compounds will provide basic information in thermodynamic assessments of binary, ternary and higher-order organic systems or organic-inorganic systems.

Keywords organics, SL model, thermodynamic properties

1. Introduction

Organic compounds are widely used in chemical industry, biotechnology, and medical applications.^[1] For example, tri- and tetra-ethylene glycols were mainly used as drying agents for natural gas, as humectants, as solvents, and in the manufacture of vinyl plasticizers.^[1,2] Phase diagram and thermodynamic database are effective tools for developing new materials, and are widely applied in inorganic systems. Now, more and more attention has been paid to that of organic systems.

Recently, some thermodynamic theories and models in the organic and polymer systems have been proposed, such as the Sanchez-Lacombe (SL) model,^[3] the Flory-Huggins model,^[4] the Universal quasi-chemical activity coefficient (UNIQUAC) model,^[5,6] etc. The Flory-Huggins model is most widely used because of its simplification; however, it is not available for vapor phase. The universal quasi-chemical activity coefficient (UNIQUAC) model is more accurate, but it is also more complex. The Sanchez-Lacombe model can be used to calculate the vapor phase because the holes of the fluid are considered, and it is not as complex as the UNIQUAC model. The main purpose of our work is to establish a more integrated and valid database of organic system. Therefore, in the present paper the Sanchez-Lacombe model is used for calculating the reduced Gibbs free energies of both liquid and vapor phases of pure organic compounds.

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2. Sanchez-Lacombe Model

The SL model^[3] was proposed by Sanchez and Lacombe based on an Ising fluid theory. Some details of this model are presented as follows.

Gibbs free energy (G) can be expressed as:

$$G = E + PV - kT \ln \Omega, \quad (\text{Eq 1})$$

where E is the configurational (potential) energy, V is the volume of a system, Ω is the number of configurations, T is the absolute temperature, and P the pressure.

In order to determine Ω , a simple case of dimers and holes on a rectangular lattice is considered.^[7] A schematic diagram of organic molecules ($r = 3$) is shown in Fig. 1. Guggenheim^[8,9] proposed an approximate method to calculate the value of Ω for a multicomponent mixture of r -mers on a lattice:

$$\Omega = \left(\frac{\delta}{\sigma} \right)^N \frac{N_r!}{N_0!N!} \left(\frac{N_q!}{N_r!} \right)^{z/2} \quad (\text{Eq 2})$$

where

$$N_r = N_0 + rN \quad (\text{Eq 3})$$

$$N_q = N_0 + qN \quad (\text{Eq 4})$$

and

$$q' = qz = (r - 2)(z - 2) + 2(z - 1). \quad (\text{Eq 5})$$

where σ is the symmetry number and δ is the flexibility parameter of a r -mer for a molecule system with N r -mers and N_0 vacant lattices, and these parameters are assumed to be independent of temperature and pressure. z is the coordination number of the lattice. Since q' is the number of the nearest nonbonded neighbors of each r -mer, q is the average neighbors of each r -mer per coordination. The total number of the nearest neighbor pairs in the system is $(z/2)N_r$, and $(z/2)N_q$ are nonbonded pairs.

Using Stirling's approximation to Eq 2, the following limiting can be obtained:

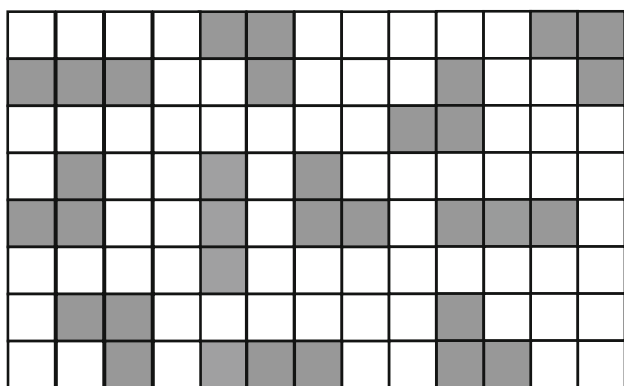


Fig. 1 Schematic diagram of organic molecules ($r = 3$). \square : Vacant lattice; \blacksquare : organic molecule

$$\lim_{z \rightarrow \infty} \Omega = \left(\frac{1}{f_0}\right)^{N_0} \left(\frac{\omega}{f}\right)^N \quad (\text{Eq 6})$$

$$\omega \equiv \frac{\delta r}{\sigma e^{r-1}} \quad (\text{Eq 7})$$

and

$$f_0 = N_0/N_r, \quad f = rN/N_r \quad (\text{Eq 8})$$

where ω is the number of configurations available to a r -mer in the close-packed pure state,^[10] f_0 is the empty site fraction, and f is the fraction of occupied sites. ω^N represents the number of ways in which N r -mers can be arranged on rN lattices (a full-filled lattice) as $z \rightarrow \infty$.^[11]

The energy of the lattice depends on the nearest neighbor interactions.^[3] Thus, the configurational (potential) energy E can be written as

$$E = -N_r \varepsilon^* f^2 \quad (\text{Eq 9})$$

where ε^* is the nonbonded, total interaction energy per mer, and it can also be regarded as the energy required to create a lattice vacancy. According to Eq 8 and 9, the following equation can be derived:

$$E = rN\varepsilon^*f \quad (\text{Eq 10})$$

Gibbs free energy in dimensionless variables (called as the reduced Gibbs free energy), \tilde{G} , can be expressed as:

$$\tilde{G} \equiv G/(Nr\varepsilon^*). \quad (\text{Eq 11})$$

According to Eq 1-10, Eq 11 can be written as:

$$\begin{aligned} \tilde{G} &= \left[-rN\varepsilon^*f + \tilde{P} \frac{\varepsilon^*}{v^*} \cdot \tilde{v}rNv^* - \tilde{T}\varepsilon^*rN \right. \\ &\quad \left. \cdot \left(\frac{f_0}{f} \ln \frac{1}{f_0} + \frac{N}{rN} \ln \frac{\omega}{f} \right) \right] / (Nr\varepsilon^*) \\ &= -\tilde{\rho} + \tilde{P}\tilde{v} + \tilde{T} \left[(\tilde{v} - 1) \ln(1 - \tilde{\rho}) + \frac{1}{r} \ln(\tilde{\rho}/\omega) \right] \quad (\text{Eq 12}) \end{aligned}$$

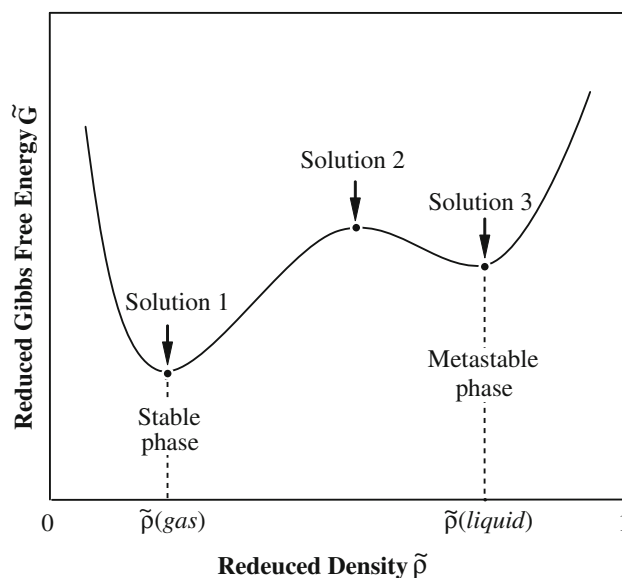


Fig. 2 Schematic of variation of the reduced Gibbs free energy \tilde{G} with reduced density at given pressure and temperature, where $\tilde{\rho}(\text{gas})$ and $\tilde{\rho}(\text{liquid})$ represent the reduced density of vapor and liquid phase, respectively

where \tilde{T} , \tilde{P} , \tilde{v} , and $\tilde{\rho}$ are the reduced temperature, pressure, volume, and density, respectively.

$$\tilde{T} \equiv T/T^*, \quad T^* \equiv \varepsilon^*/k \quad (\text{Eq 13})$$

$$\tilde{P} \equiv P/P^*, \quad P^* \equiv \varepsilon^*/v^* \quad (\text{Eq 14})$$

and

$$\tilde{v} \equiv \frac{1}{\tilde{\rho}} \equiv V/V^* \equiv \frac{1}{f}, \quad V^* = N(rv^*) \quad (\text{Eq 15})$$

where v^* , r , and ε^* are molecular parameters, which completely characterize a pure fluid.

3. Method of Calculation

The extremum of the reduced Gibbs free energy is obtained in the usual way:

$$\left. \frac{\partial \tilde{G}}{\partial \tilde{v}} \right|_{\tilde{T}, \tilde{P}} = 0, \quad (\text{Eq 16})$$

which yields the equation of state,

$$\tilde{\rho}^2 + \tilde{P} + \tilde{T} \left[\ln(1 - \tilde{\rho}) + \left(1 - \frac{1}{r}\right) \tilde{\rho} \right] = 0. \quad (\text{Eq 17})$$

At given \tilde{T} and \tilde{P} , there are three solutions in Eq 17, as shown in Fig. 2. The highest density $\tilde{\rho}$ (liquid) corresponds to a liquid phase, while the lowest density $\tilde{\rho}$ (gas) corresponds to a vapor phase. By comparing the reduced

Table 1 Data on pure organic properties

No.	CAS number	Name	Formula	Formula weight	ϵ^* , kJ mol ⁻¹	v^* , cm ³ mol ⁻¹	r	Melting point, T_m , K	Boiling point, T_b , K	
									Ref. [12]	Calculated
1	75-83-2	2,2-Dimethylbutane	CH ₃ CH ₂ C(CH ₃) ₃	86.18	3.797	13.77	8.1	173.6	323.2	323.7
2	75-29-8	2,3-Dimethylbutane	(CH ₃) ₂ CHCH(CH ₃) ₂	86.18	3.864	13.31	8.29	145	331.5	331.8
3	71-43-2	Benzene	C ₆ H ₆	78.11	4.364	9.8	8.02	279	353.5	353.9
4	56-23-5	Carbon tetrachloride	CCl ₄	153.82	4.469	11.69	7.36	250.5	350.2	351
5	108-90-7	Chlorobenzene	C ₆ H ₅ Cl	112.56	4.88	11.14	8.38	228.2	405.2	405.7
6	75-15-0	Carbon disulfide	CS ₂	76.14	4.729	9.15	5.95	161.9	320	319.9
7	110-82-7	Cyclohexane	C ₆ H ₁₂	84.16	4.145	10.79	8.65	280.1	354.2	354.6
8	287-92-3	Cyclopentane	C ₅ H ₁₀	70.13	4.019	10.53	7.68	179.5	322.8	323.1
9	74-84-0	Ethane	CH ₃ CH ₃	30.07	2.633	8	5.87	90.7	185.5	184.7
10	75-28-5	Isobutane	(CH ₃) ₂ CHCH ₃	58.12	3.322	11.49	7.03	135.5	261.8	261.4
11	74-82-8	Methane	CH ₄	16.04	1.873	7.52	4.26	91	112	111.4
12	75-09-2	Dichloromethane	CH ₂ Cl ₂	84.93	4.061	7.23	7.64	178.5	313.5	314.2
13	108-38-3	<i>m</i> -Xylene	C ₆ H ₄ (CH ₃) ₂	106.17	4.679	12.11	9.21	225.6	412.5	413
14	106-97-8	Butane	CH ₃ CH ₂ CH ₂ CH ₃	58.12	3.368	10.4	7.59	135.2	273	273.3
15	1120-21-4	Undecane	CH ₃ (CH ₂) ₉ CH ₃	156.31	4.523	14.89	12.4	247.9	469.5	470.1
16	112-40-3	Dodecane	CH ₃ (CH ₂) ₁₀ CH ₃	170.34	4.612	15.28	13.06	263.5	489.7	490.7
17	629-50-5	Tridecane	CH ₃ (CH ₂) ₁₁ CH ₃	184.37	4.675	15.58	13.79	269	508.5	509.6
18	629-59-4	Tetradecane	CH ₃ (CH ₂) ₁₂ CH ₃	198.4	4.754	15.99	14.36	279	527.1	527.8
19	629-78-7	Heptadecane	CH ₃ (CH ₂) ₁₅ CH ₃	240.41	4.973	17.26	15.83	295.5	575.7	576.4
20	124-18-5	Decane	CH ₃ (CH ₂) ₈ CH ₃	142.29	4.423	14.47	11.75	243.8	447.6	448.3
21	463-82-1	Neopentane	(CH ₃) ₄ C	72.15	3.461	12.97	7.47	256.9	283	283.6
22	142-82-5	Heptane	CH ₃ (CH ₂) ₅ CH ₃	100.21	4.061	13.09	9.57	182.9	371.9	372.8
23	110-54-3	Hexane	CH ₃ (CH ₂) ₄ CH ₃	86.18	3.977	13.28	8.37	178.1	342.2	342.3
24	111-84-2	Nonane	CH ₃ (CH ₂) ₇ CH ₃	128.26	4.313	14	11.06	220	424.3	424.8
25	111-65-9	Octane	CH ₃ (CH ₂) ₆ CH ₃	114.23	4.192	13.55	10.34	216.7	399.2	399.7
26	109-66-0	Pentane	CH ₃ (CH ₂) ₃ CH ₃	72.15	3.679	11.82	8.09	143.8	309.5	309.9
27	95-47-6	<i>o</i> -Xylene	C ₆ H ₄ (CH ₃) ₂	106.17	4.767	12.03	9.14	248.3	418	418.2
28	74-98-6	Propane	CH ₃ CH ₂ CH ₃	44.1	3.095	9.84	6.5	85.5	231.4	231.2
29	106-42-3	<i>p</i> -Xylene	C ₆ H ₄ (CH ₃) ₂	106.17	4.683	12.24	9.14	286.5	411.5	412.2
30	108-88-3	Toluene	C ₆ H ₅ CH ₃	92.14	4.536	11.22	8.5	178.6	384.1	382.7

Gibbs free energies corresponding to \tilde{p} (liquid) and \tilde{p} (gas), it is known that the lowest \tilde{G} corresponds to the stable phase. In Fig. 2, the gas phase is stable with respect to the liquid phase at the given pressure and temperature.

According to Eq 17, in the case of $P = 1$ atm, the reduced densities of both liquid phase and vapor phase at different temperatures are calculated by means of the molecular parameters (v^* , r , and ϵ^*) as shown in Table 1. The expressions of \tilde{p} (liquid) and \tilde{p} (gas) with the dependence of temperature can be derived by polyfitting these data.

Furthermore, as it can be seen from Eq 17, ω is of no consequence for the equation of state,^[3] because it is assumed to be constant. The entropy can be derived from the number of configurations, as follows:

$$S = k \ln \Omega. \quad (\text{Eq 18})$$

According to Eq 6-8, the parameter ω can be estimated using the entropies at 298 K:

$$S_{298} = -krN \left[(\tilde{v} - 1) \ln(1 - \tilde{p}) + \frac{1}{r} \ln(\tilde{p}/\omega) \right]. \quad (\text{Eq 19})$$

For 1 mole organic compounds, the following equation can be derived:

$$S_{298}^0 = -Rr \left[(\tilde{v} - 1) \ln(1 - \tilde{p}) + \frac{1}{r} \ln(\tilde{p}/\omega) \right], \quad (\text{Eq 20})$$

where R is the gas constant. According to Eq 17 and 20, the value of ω can be calculated.

Using the molecular parameters (v^* , r , and ϵ^*), the number of configurations available to a r -mer in the close-packed pure state ω , and the expressions of reduced densities, the reduced Gibbs free energy of both phases can be derived based on Eq 12.

4. Results

The information on the boiling temperature, melting temperature, molecular parameters and structure of organic compounds are summarized in Table 1. The molecular parameters (v^* , r , and ϵ^*) are mainly taken from the data reported by Sanchez and Lacombe,^[3] and the other

information are from the Lange's Handbook of Chemistry^[12] and CRC Handbook of Chemistry and Physics.^[13] The boiling points (T_b) of 30 kinds of pure organic compounds can be derived according to Eq 12 and 17. The calculated boiling points (T_b) are in good agreement with the experimental data,^[12] as presented in Table 1.

Table 2 The entropies and the calculated value of ω

No.	Name	Entropy, S_{298}^0 , $\text{J K}^{-1} \text{mol}^{-1}$		ω
		Liquid	Vapor	
1	2,2-Dimethylbutane	272.5*	358.2	$7.878 * 10^{12}$
2	2,3-Dimethylbutane	287.8*	365.8	$5.225 * 10^{13}$
3	Benzene	173.4*	269.2	$1.034 * 10^8$
		171.5 ^Δ	269.3 ^Δ	
4	Carbon tetrachloride	216.2*	309.9	$2.281 * 10^{10}$
		216.4 ^Δ	309.8 ^Δ	
5	Chlorobenzene	209.2*		$1.114 * 10^{10}$
6	Carbon disulfide	151 ^{Δ,*}	238 ^Δ	$1.504 * 10^7$
7	Cyclohexane	204.4*	298.3	$2.924 * 10^9$
		204.3 ^Δ		
8	Cyclopentane	204.3*	292.9	$3.232 * 10^9$
9	Ethane		229.1*	$6.399 * 10^6$
			229.6	
10	Isobutane		294.6*	$7.366 * 10^9$
11	Methane		186.3*	$4.283 * 10^5$
12	Dichloromethane	177.8*	270.3	$1.411 * 10^8$
13	<i>m</i> -Xylene	252.2*	357.7	$1.382 * 10^{12}$
14	Butane		310.1	$2.603 * 10^{10}$
15	Undecane	458.1*		$3.2 * 10^{22}$
16	Dodecane	490.6*	622.5	$1.418 * 10^{24}$
17	Tridecane		661.5*	$3.636 * 10^{26}$
18	Tetradecane		700.4*	$2.43 * 10^{28}$
19	Heptadecane		813.1*	$4.947 * 10^{33}$
20	Decane	425.5*	544.7	$6.583 * 10^{20}$
		425.9 ^Δ		
21	Neopentane		306.4	$2.337 * 10^{10}$
22	Heptane	328.6 ^{Δ,*}	427.9	$6.328 * 10^{15}$
			428 ^Δ	
23	Hexane	296.1*	388.4	$1.58 * 10^{14}$
		292.5 ^Δ	388.5 ^Δ	
24	Nonane	393.7 ^{Δ,*}	505.7*	$1.486 * 10^{19}$
			505.8 ^Δ	
25	Octane	361.2 ^{Δ,*}	466.7	$3.083 * 10^{17}$
			466.8 ^Δ	
26	Pentane	262.7*	349	$2.091 * 10^{12}$
		259.9 ^Δ	349.1 ^Δ	
27	<i>o</i> -Xylene	246.5*	352.8	$7.656 * 10^{11}$
28	Propane		270.2*	$5.412 * 10^8$
			270 ^Δ	
29	<i>p</i> -Xylene	247.4*	352.4	$7.9 * 10^{11}$
30	Toluene	221*	320.7	$3.373 * 10^{10}$

Data with "Δ" are taken from Ref. ^[13], and others are from Ref. ^[11]

Data with "*" are adopted in this paper

These data are applicable at 1 atm

Table 2 shows the entropies of each organic compound, including both liquid and vapor phase. These data are mainly from the Lange's Handbook of Chemistry^[12] and Thermochemical Data of Elements and Compounds.^[14] By considering the entropy at 298 K, the value of ω of each compound is estimated based on Eq 20, and is also presented in Table 2.

The reduced Gibbs free energy \tilde{G} of 30 kinds of pure organic compounds are calculated according to Eq 12 and 17, using the molecular parameters (v^* , r , and ϵ^*) and ω . The diagrams of reduced Gibbs free energies at $P = 1$ atm are shown in Appendix, including the expression of reduced Gibbs free energies and the reduced densities of both liquid and vapor phases with the dependence of temperature. The ranges of temperature in which the given phases are stable are also presented in Appendix.

5. Summary

The Gibbs free energies of 30 kinds of pure organic compounds are calculated based on the SL model. The calculated boiling points (T_b) of pure organic compounds are in good agreement with the experimental data. It is hoped that this database will become important basic information in thermodynamic assessments of organic systems.

Acknowledgment

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6. Appendix: Summary of Calculated Thermodynamic Properties of Pure Organic Compounds ($P = 1$ atm)

6.1 (1) 2,2-Dimethylbutane

The reduced Gibbs free energy \tilde{G} for 2,2-dimethylbutane

$$\tilde{G} = -\tilde{p} + 3.6267 \times 10^{-4} / \tilde{p} + 0.0022T((1/\tilde{p} - 1) \times \ln(1 - \tilde{p}) + 0.1235 \ln(\tilde{p}) - 3.6673)$$

where

$$\begin{aligned} \tilde{p}(\text{liquid}) &= 0.9961 + 2.90491 \times 10^{-4}T - 2.79447 \\ &\quad \times 10^{-6}T^2 \quad 173.6 \text{ K} < T < 323.7 \text{ K} \\ \tilde{p}(\text{gas}) &= 0.01487 - 5.09615 \times 10^{-5}T + 5.63889 \\ &\quad \times 10^{-8}T^2 \quad T > 323.7 \text{ K} \end{aligned}$$

6.2 (2) 2,3-Dimethylbutane

The reduced Gibbs free energy \tilde{G} for 2,3-dimethylbutane

$$\tilde{G} = -\tilde{p} + 3.4446 \times 10^{-4} / \tilde{p} + 0.0022T((1/\tilde{p} - 1) \times \ln(1 - \tilde{p}) + 0.1206 \ln(\tilde{p}) - 3.8094)$$

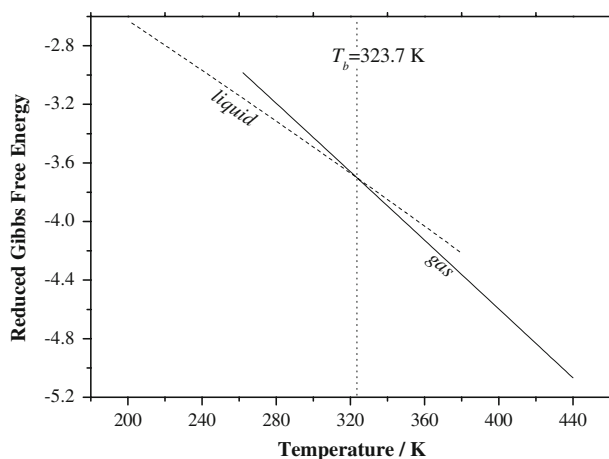


Fig. A1 Reduced Gibbs free energy of 2,2-dimethylbutane

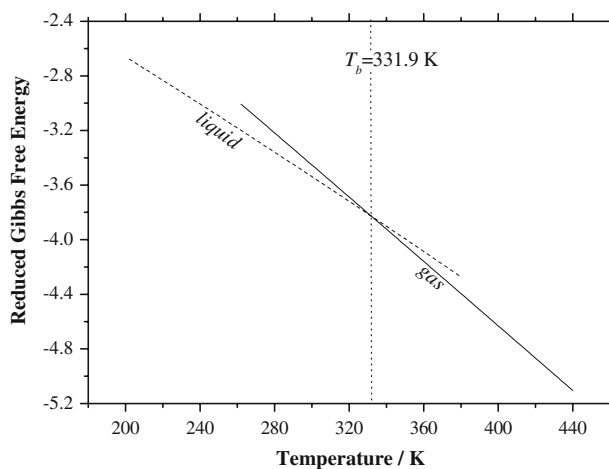


Fig. A2 Reduced Gibbs free energy of 2,3-dimethylbutane

where

$$\begin{aligned} \tilde{p}(\text{liquid}) &= 0.99449 + 2.95294 \times 10^{-4}T \\ &\quad - 2.7029 \times 10^{-6}T^2 \quad 145 \text{ K} < T < 331.9 \text{ K} \\ \tilde{p}(\text{gas}) &= 0.01416 - 4.69273 \times 10^{-5}T \\ &\quad + 5.02457 \times 10^{-8}T^2 \quad T > 331.9 \text{ K} \end{aligned}$$

6.3 (3) Benzene

The reduced Gibbs free energy \tilde{G} for benzene

$$\begin{aligned} \tilde{G} &= -\tilde{p} + 2.2457 \times 10^{-4}/\tilde{p} + 0.0019T((1/\tilde{p} - 1) \\ &\quad \times \ln(1 - \tilde{p}) + 0.1247 \ln(\tilde{p}) - 2.3012) \end{aligned}$$

where

$$\begin{aligned} \tilde{p}(\text{liquid}) &= 0.99426 + 2.64734 \times 10^{-4}T \\ &\quad - 2.13832 \times 10^{-6}T^2 \quad 279 \text{ K} < T < 353.9 \text{ K} \\ \tilde{p}(\text{gas}) &= 0.00877 - 2.59175 \times 10^{-5}T \\ &\quad + 2.50225 \times 10^{-8}T^2 \quad T > 353.9 \text{ K} \end{aligned}$$

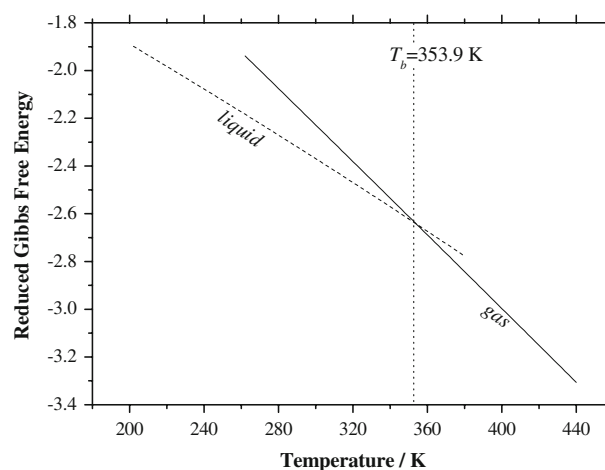


Fig. A3 Reduced Gibbs free energy of benzene

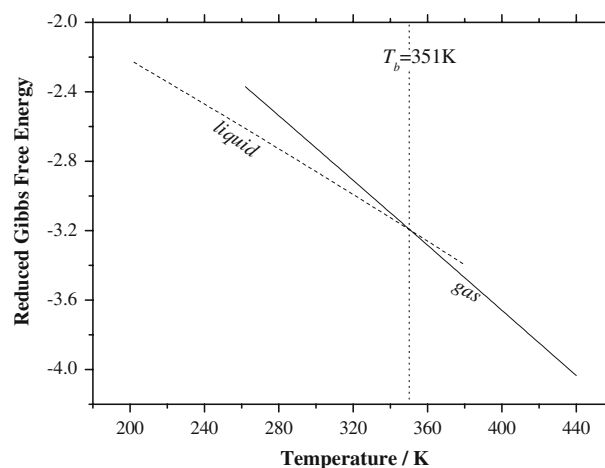


Fig. A4 Reduced Gibbs free energy of CCl₄

6.4 (4) CCl₄

The reduced Gibbs free energy \tilde{G} for CCl₄

$$\begin{aligned} \tilde{G} &= -\tilde{p} + 2.6159 \times 10^{-4}/\tilde{p} + 0.0019T((1/\tilde{p} - 1) \\ &\quad \times \ln(1 - \tilde{p}) + 0.1359 \ln(\tilde{p}) - 3.2413) \end{aligned}$$

where

$$\begin{aligned} \tilde{p}(\text{liquid}) &= 0.99304 + 2.78589 \times 10^{-4}T \\ &\quad - 2.11556 \times 10^{-6}T^2 \quad 250.5 \text{ K} < T < 351 \text{ K} \\ \tilde{p}(\text{gas}) &= 0.00998 - 3.05005 \times 10^{-5}T \\ &\quad + 3.0387 \times 10^{-8}T^2 \quad T > 351 \text{ K} \end{aligned}$$

6.5 (5) Chlorobenzene

The reduced Gibbs free energy \tilde{G} for chlorobenzene

$$\begin{aligned} \tilde{G} &= -\tilde{p} + 2.32019 \times 10^{-4}/\tilde{p} + 0.001709T((1/\tilde{p} - 1) \\ &\quad \times \ln(1 - \tilde{p}) + 0.11933 \ln(\tilde{p}) - 2.7606) \end{aligned}$$

where

$$\begin{aligned} \tilde{\rho}(\text{liquid}) &= 0.99787 + 2.11252 \times 10^{-4}T \\ &\quad - 1.65643 \times 10^{-6}T^2 \quad 228.2 \text{ K} < T < 405.7 \text{ K} \\ \tilde{\rho}(\text{gas}) &= 0.00917 - 2.3815 \times 10^{-5}T \\ &\quad + 2.01886 \times 10^{-8}T^2 \quad T > 405.7 \text{ K} \end{aligned}$$

6.6 (6) CS₂

The reduced Gibbs free energy \tilde{G} for CS₂

$$\begin{aligned} \tilde{G} &= -\tilde{\rho} + 1.9348 \times 10^{-4}/\tilde{\rho} + 0.0018T((1/\tilde{\rho} - 1) \\ &\quad \times \ln(1 - \tilde{\rho}) + 0.1681 \ln(\tilde{\rho}) - 2.7781) \end{aligned}$$

where

$$\begin{aligned} \tilde{\rho}(\text{liquid}) &= 0.98647 + 3.36423 \times 10^{-4}T \\ &\quad - 2.11733 \times 10^{-6}T^2 \quad 161.9 \text{ K} < T < 319.9 \text{ K} \\ \tilde{\rho}(\text{gas}) &= 0.00669 - 2.20176 \times 10^{-5}T \\ &\quad + 2.37727 \times 10^{-8}T^2 \quad T > 319.9 \text{ K} \end{aligned}$$

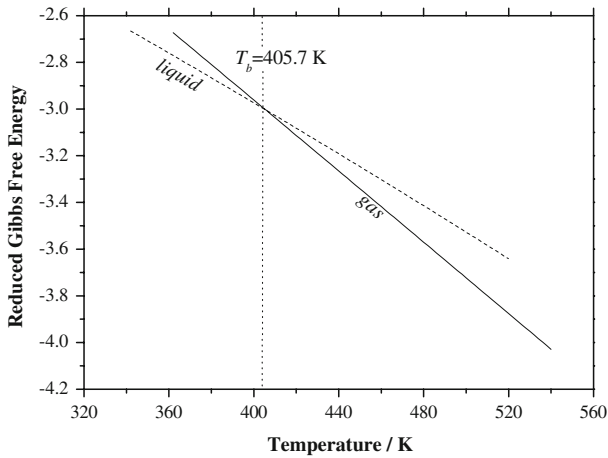


Fig. A5 Reduced Gibbs free energy of chlorobenzene

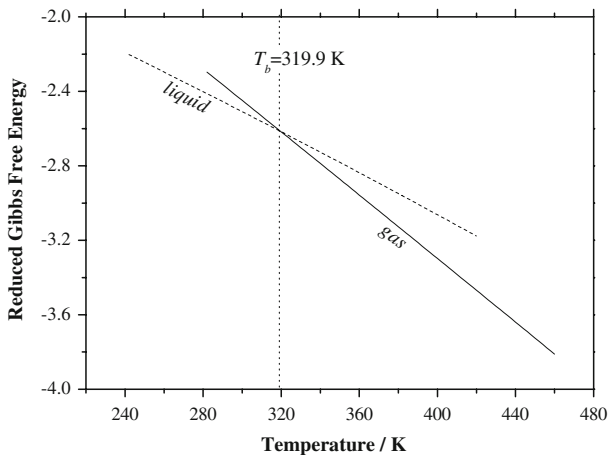


Fig. A6 Reduced Gibbs free energy of CS₂

6.7 (7) Cyclohexane

The reduced Gibbs free energy \tilde{G} for cyclohexane

$$\begin{aligned} \tilde{G} &= -\tilde{\rho} + 2.6029 \times 10^{-4}/\tilde{\rho} + 0.0020T((1/\tilde{\rho} - 1) \\ &\quad \times \ln(1 - \tilde{\rho}) + 0.1156 \ln(\tilde{\rho}) - 2.5196) \end{aligned}$$

where

$$\begin{aligned} \tilde{\rho}(\text{liquid}) &= 0.99409 + 2.67991 \times 10^{-4}T \\ &\quad - 2.30746 \times 10^{-6}T^2 \quad 280.1 \text{ K} < T < 354.6 \text{ K} \\ \tilde{\rho}(\text{gas}) &= 0.01045 - 3.07275 \times 10^{-5}T \\ &\quad + 2.94078 \times 10^{-8}T^2 \quad T > 354.6 \text{ K} \end{aligned}$$

6.8 (8) Cyclopentane

The reduced Gibbs free energy \tilde{G} for cyclopentane

$$\begin{aligned} \tilde{G} &= -\tilde{\rho} + 2.66667 \times 10^{-4}/\tilde{\rho} + 0.002037T((1/\tilde{\rho} - 1) \\ &\quad \times \ln(1 - \tilde{\rho}) + 0.130208 \ln(\tilde{\rho}) - 2.8511) \end{aligned}$$

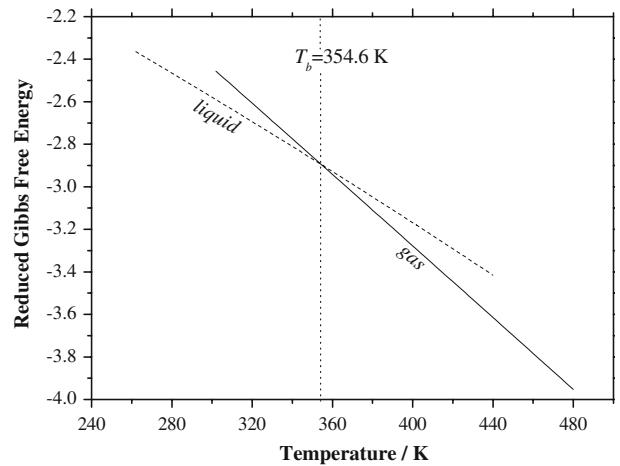


Fig. A7 Reduced Gibbs free energy of cyclohexane

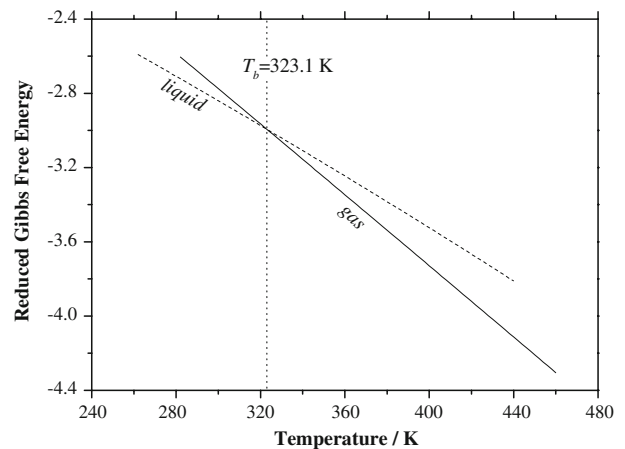


Fig. A8 Reduced Gibbs free energy of cyclopentane

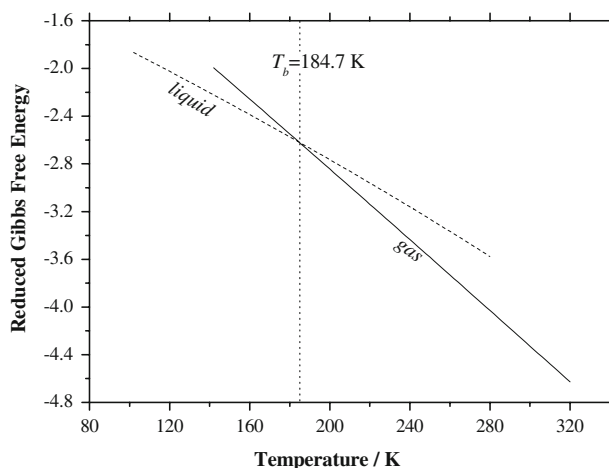


Fig. A9 Reduced Gibbs free energy of ethane

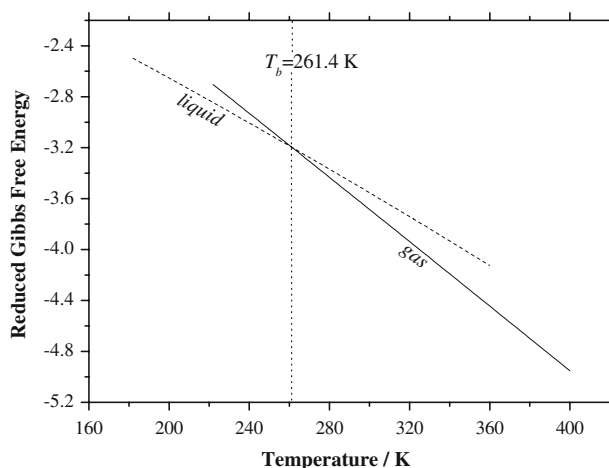


Fig. A10 Reduced Gibbs free energy of isobutane

where

$$\begin{aligned} \tilde{\rho}(\text{liquid}) &= 0.99461 + 2.93188 \times 10^{-4}T \\ &\quad - 2.56055 \times 10^{-6}T^2 \quad 179.5 \text{ K} < T < 323.1 \text{ K} \\ \tilde{\rho}(\text{gas}) &= 0.01034 - 3.47535 \times 10^{-5}T \\ &\quad + 3.79926 \times 10^{-8}T^2 \quad T > 323.1 \text{ K} \end{aligned}$$

6.9 (9) Ethane

The reduced Gibbs free energy \tilde{G} for ethane

$$\tilde{G} = -\tilde{\rho} + 3.0379 \times 10^{-4}/\tilde{\rho} + 0.0032T((1/\tilde{\rho} - 1) \times \ln(1 - \tilde{\rho}) + 0.1704 \ln(\tilde{\rho}) - 2.6704)$$

where

$$\begin{aligned} \tilde{\rho}(\text{liquid}) &= 0.98542 + 6.22432 \times 10^{-4}T \\ &\quad - 6.91278 \times 10^{-6}T^2 \quad 90.7 \text{ K} < T < 184.7 \text{ K} \\ \tilde{\rho}(\text{gas}) &= 0.01022 - 5.84055 \times 10^{-5}T \\ &\quad + 1.08376 \times 10^{-7}T^2 \quad T > 184.7 \text{ K} \end{aligned}$$

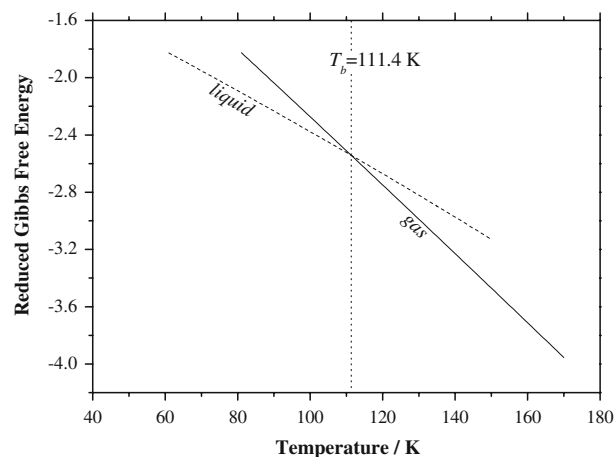


Fig. A11 Reduced Gibbs free energy of methane

6.10 (10) Isobutane

The reduced Gibbs free energy \tilde{G} for isobutane

$$\tilde{G} = -\tilde{\rho} + 3.4586 \times 10^{-4}/\tilde{\rho} + 0.0025T((1/\tilde{\rho} - 1) \times \ln(1 - \tilde{\rho}) + 0.1422 \ln(\tilde{\rho}) - 3.2308)$$

where

$$\begin{aligned} \tilde{\rho}(\text{liquid}) &= 0.99068 + 4.07649 \times 10^{-4}T \\ &\quad - 3.9513 \times 10^{-6}T^2 \quad 135.5 \text{ K} < T < 261.4 \text{ K} \\ \tilde{\rho}(\text{gas}) &= 0.01241 - 4.98141 \times 10^{-5}T \\ &\quad + 6.48941 \times 10^{-8}T^2 \quad T > 261.4 \text{ K} \end{aligned}$$

6.11 (11) Methane

The reduced Gibbs free energy \tilde{G} for methane

$$\tilde{G} = -\tilde{\rho} + 4.0145 \times 10^{-4}/\tilde{\rho} + 0.0044T((1/\tilde{\rho} - 1) \times \ln(1 - \tilde{\rho}) + 0.2347 \ln(\tilde{\rho}) - 3.0435)$$

where

$$\begin{aligned} \tilde{\rho}(\text{liquid}) &= 0.95195 + 0.001717T \\ &\quad - 1.91379 \times 10^{-5}T^2 \quad 91 \text{ K} < T < 111.4 \text{ K} \\ \tilde{\rho}(\text{gas}) &= 0.01036 - 8.78482 \times 10^{-5}T \\ &\quad + 2.40536 \times 10^{-7}T^2 \quad T > 111.4 \text{ K} \end{aligned}$$

6.12 (12) Methylene chloride

The reduced Gibbs free energy \tilde{G} for methylene chloride

$$\tilde{G} = -\tilde{\rho} + 1.7802 \times 10^{-4}/\tilde{\rho} + 0.0020T((1/\tilde{\rho} - 1) \times \ln(1 - \tilde{\rho}) + 0.1309 \ln(\tilde{\rho}) - 2.4563)$$

where

$$\begin{aligned} \tilde{\rho}(\text{liquid}) &= 0.9944 + 2.91766 \times 10^{-4}T \\ &\quad - 2.51292 \times 10^{-6}T^2 \quad 178.5 \text{ K} < T < 314.2 \text{ K} \\ \tilde{\rho}(\text{gas}) &= 0.00683 - 2.25368 \times 10^{-5}T \\ &\quad + 2.43825 \times 10^{-8}T^2 \quad T > 314.2 \text{ K} \end{aligned}$$

6.13 (13) *m*-Xylene

The reduced Gibbs free energy \tilde{G} for *m*-xylene

$$\tilde{G} = -\tilde{\rho} + 2.5883 \times 10^{-4}/\tilde{\rho} + 0.0018T((1/\tilde{\rho} - 1) \times \ln(1 - \tilde{\rho}) + 0.1086 \ln(\tilde{\rho}) - 3.0359)$$

where

$$\begin{aligned} \tilde{\rho}(\text{liquid}) &= 1.00111 + 1.89322 \times 10^{-4}T \\ &\quad - 1.71662 \times 10^{-6}T^2 \quad 225.6 \text{ K} < T < 413 \text{ K} \\ \tilde{\rho}(\text{gas}) &= 0.01088 - 2.78382 \times 10^{-5}T \\ &\quad + 2.31598 \times 10^{-8}T^2 \quad T > 413 \text{ K} \end{aligned}$$

6.14 (14) *n*-Butane

The reduced Gibbs free energy \tilde{G} for *n*-butane

$$\tilde{G} = -\tilde{\rho} + 3.0875 \times 10^{-4}/\tilde{\rho} + 0.0025T((1/\tilde{\rho} - 1) \times \ln(1 - \tilde{\rho}) + 0.1318 \ln(\tilde{\rho}) - 3.1609)$$

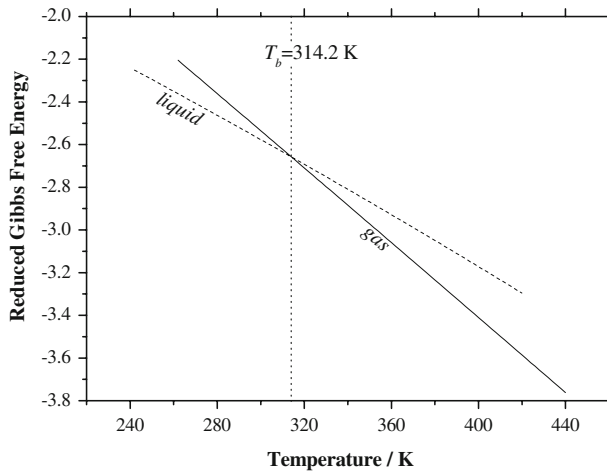


Fig. A12 Reduced Gibbs free energy of methylene chloride

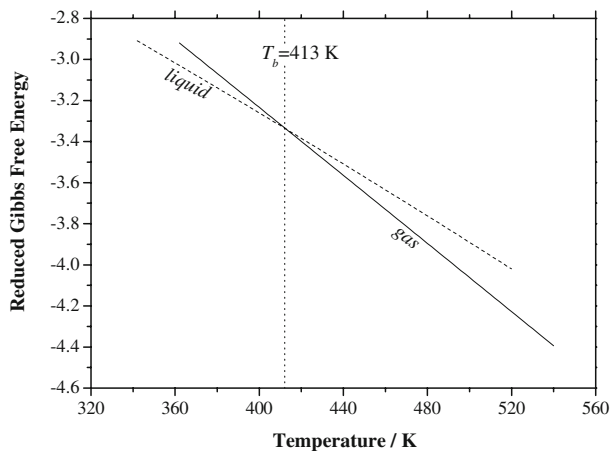


Fig. A13 Reduced Gibbs free energy of *m*-xylene

where

$$\begin{aligned} \tilde{\rho}(\text{liquid}) &= 0.99348 + 3.62032 \times 10^{-4}T \\ &\quad - 3.6825 \times 10^{-6}T^2 \quad 135.2 \text{ K} < T < 273.3 \text{ K} \\ \tilde{\rho}(\text{gas}) &= 0.01166 - 4.50511 \times 10^{-5}T \\ &\quad + 5.65292 \times 10^{-8}T^2 \quad T > 273.3 \text{ K} \end{aligned}$$

6.15 (15) *n*-C₁₁H₂₄

The reduced Gibbs free energy \tilde{G} for *n*-C₁₁H₂₄

$$\tilde{G} = -\tilde{\rho} + 3.2918 \times 10^{-4}/\tilde{\rho} + 0.0018T((1/\tilde{\rho} - 1) \times \ln(1 - \tilde{\rho}) + 0.0806 \ln(\tilde{\rho}) - 4.1792)$$

where

$$\begin{aligned} \tilde{\rho}(\text{liquid}) &= 0.99048 + 2.10935 \times 10^{-4}T \\ &\quad - 1.72686 \times 10^{-6}T^2 \quad 247.9 \text{ K} < T < 470.1 \text{ K} \\ \tilde{\rho}(\text{gas}) &= 0.01685 - 3.89705 \times 10^{-5}T \\ &\quad + 2.89231 \times 10^{-8}T^2 \quad T > 470.1 \text{ K} \end{aligned}$$

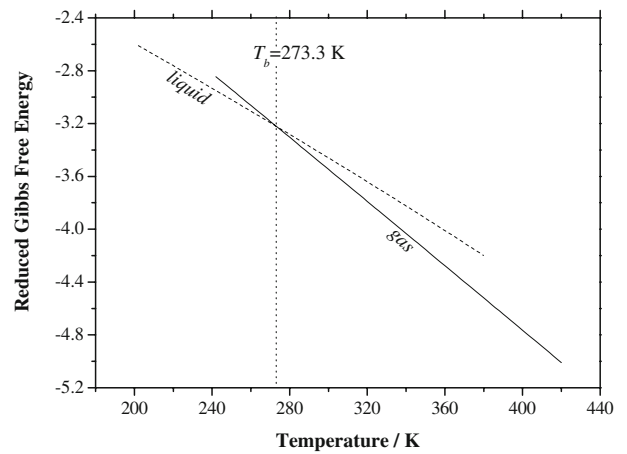


Fig. A14 Reduced Gibbs free energy of *n*-butane

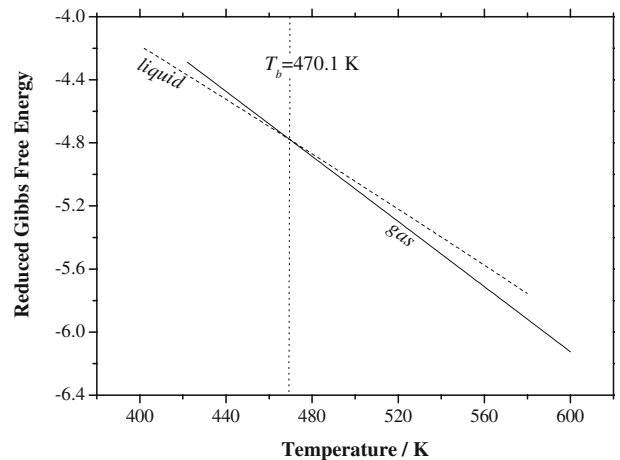


Fig. A15 Reduced Gibbs free energy of *n*-C₁₁H₂₄

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6.16 (16) $n\text{-C}_{12}\text{H}_{26}$

The reduced Gibbs free energy \tilde{G} for $n\text{-C}_{12}\text{H}_{26}$

$$\tilde{G} = -\tilde{\rho} + 3.3134 \times 10^{-4} / \tilde{\rho} + 0.0018T((1/\tilde{\rho} - 1) \times \ln(1 - \tilde{\rho}) + 0.0766 \ln(\tilde{\rho}) - 4.2598)$$

where

$$\begin{aligned} \tilde{\rho}(\text{liquid}) &= 0.9775 + 2.5113 \times 10^{-4}T \\ &\quad - 1.68175 \times 10^{-6}T^2 \quad 263.5 \text{ K} < T < 490.7 \text{ K} \\ \tilde{\rho}(\text{gas}) &= 0.01886 - 4.43174 \times 10^{-5}T \\ &\quad + 3.32017 \times 10^{-8}T^2 \quad T > 490.7 \text{ K} \end{aligned}$$

6.17 (17) $n\text{-C}_{13}\text{H}_{28}$

The reduced Gibbs free energy \tilde{G} for $n\text{-C}_{13}\text{H}_{28}$

$$\tilde{G} = -\tilde{\rho} + 3.3329 \times 10^{-4} / \tilde{\rho} + 0.0018T((1/\tilde{\rho} - 1) \times \ln(1 - \tilde{\rho}) + 0.0725 \ln(\tilde{\rho}) - 4.434)$$

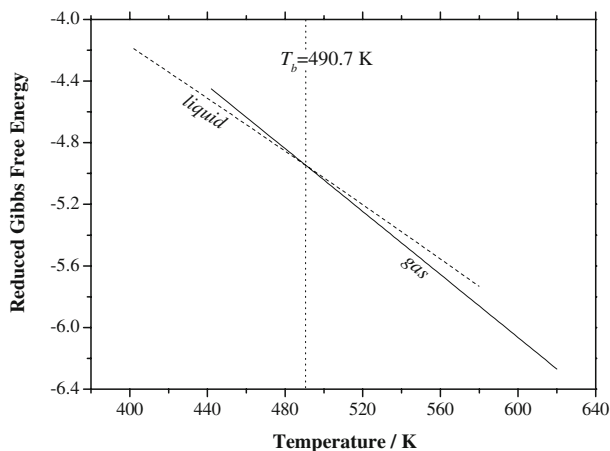


Fig. A16 Reduced Gibbs free energy of $n\text{-C}_{12}\text{H}_{26}$

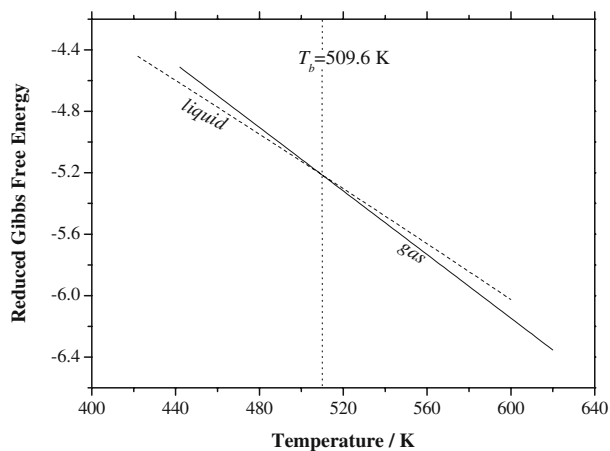


Fig. A17 Reduced Gibbs free energy of $n\text{-C}_{13}\text{H}_{28}$

where

$$\begin{aligned} \tilde{\rho}(\text{liquid}) &= 0.98403 + 2.08061 \times 10^{-4}T \\ &\quad - 1.56916 \times 10^{-6}T^2 \quad 269 \text{ K} < T < 509.6 \text{ K} \\ \tilde{\rho}(\text{gas}) &= 0.01908 - 4.22023 \times 10^{-5}T \\ &\quad + 2.97498 \times 10^{-8}T^2 \quad T > 509.6 \text{ K} \end{aligned}$$

6.18 (18) $n\text{-C}_{14}\text{H}_{30}$

The reduced Gibbs free energy \tilde{G} for $n\text{-C}_{14}\text{H}_{30}$

$$\tilde{G} = -\tilde{\rho} + 3.3632 \times 10^{-4} / \tilde{\rho} + 0.0017T((1/\tilde{\rho} - 1) \times \ln(1 - \tilde{\rho}) + 0.0696 \ln(\tilde{\rho}) - 4.5491)$$

where

$$\begin{aligned} \tilde{\rho}(\text{liquid}) &= 0.97704 + 2.27337 \times 10^{-4}T \\ &\quad - 1.52527 \times 10^{-6}T^2 \quad 279 \text{ K} < T < 527.8 \text{ K} \\ \tilde{\rho}(\text{gas}) &= 0.01979 - 4.22883 \times 10^{-5}T \\ &\quad + 2.8751 \times 10^{-8}T^2 \quad T > 527.8 \text{ K} \end{aligned}$$

6.19 (19) $n\text{-C}_{17}\text{H}_{36}$

The reduced Gibbs free energy \tilde{G} for $n\text{-C}_{17}\text{H}_{36}$

$$\tilde{G} = -\tilde{\rho} + 3.4709 \times 10^{-4} / \tilde{\rho} + 0.0017T((1/\tilde{\rho} - 1) \times \ln(1 - \tilde{\rho}) + 0.0632 \ln(\tilde{\rho}) - 4.9033)$$

where

$$\begin{aligned} \tilde{\rho}(\text{liquid}) &= 0.99948 + 1.16273 \times 10^{-4}T \\ &\quad - 1.26522 \times 10^{-6}T^2 \quad 295.5 \text{ K} < T < 576.4 \text{ K} \\ \tilde{\rho}(\text{gas}) &= 0.02326 - 4.76954 \times 10^{-5}T \\ &\quad + 3.08207 \times 10^{-8}T^2 \quad T > 576.4 \text{ K} \end{aligned}$$

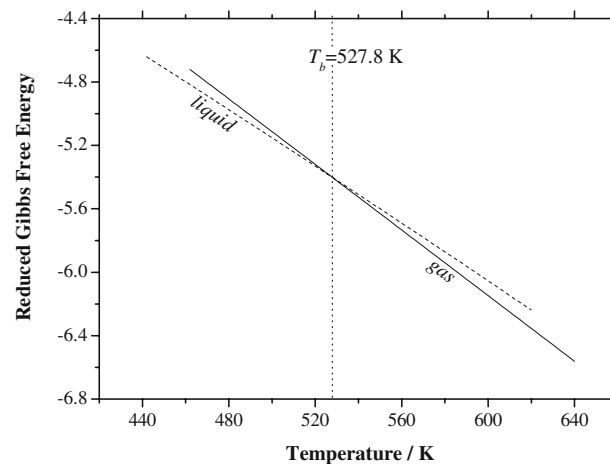


Fig. A18 Reduced Gibbs free energy of $n\text{-C}_{14}\text{H}_{30}$

6.20 (20) *n*-Decane

The reduced Gibbs free energy \tilde{G} for *n*-decane

$$\tilde{G} = -\tilde{\rho} + 3.2718 \times 10^{-4} / \tilde{\rho} + 0.0019T((1/\tilde{\rho} - 1) \times \ln(1 - \tilde{\rho}) + 0.0851 \ln(\tilde{\rho}) - 4.0794)$$

where

$$\begin{aligned} \tilde{\rho}(\text{liquid}) &= 0.9537 + 4.0064 \times 10^{-4}T \\ &\quad - 2.05117 \times 10^{-6}T^2 \quad 243.8 \text{ K} < T < 448.3 \text{ K} \\ \tilde{\rho}(\text{gas}) &= 0.01653 - 4.076 \times 10^{-5}T \\ &\quad + 3.22602 \times 10^{-8}T^2 \quad T > 448.3 \text{ K} \end{aligned}$$

6.21 (21) Neopentane

The reduced Gibbs free energy \tilde{G} for neopentane

$$\tilde{G} = -\tilde{\rho} + 3.7477 \times 10^{-4} / \tilde{\rho} + 0.0024T((1/\tilde{\rho} - 1) \times \ln(1 - \tilde{\rho}) + 0.1339 \ln(\tilde{\rho}) - 3.1968)$$

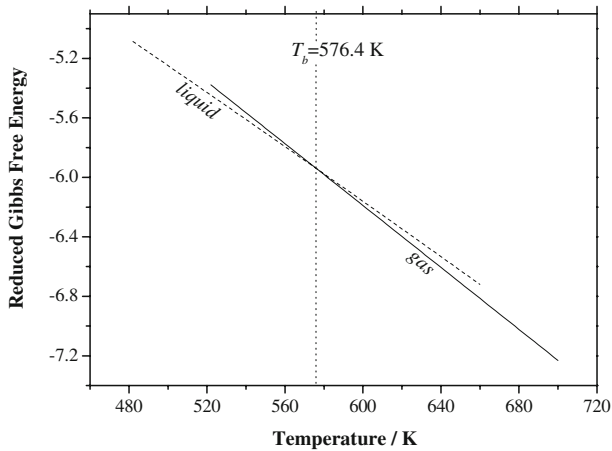


Fig. A19 Reduced Gibbs free energy of *n*-C₁₇H₃₆

where

$$\begin{aligned} \tilde{\rho}(\text{liquid}) &= 0.9383 + 7.65055 \times 10^{-4}T \\ &\quad - 4.26628 \times 10^{-6}T^2 \quad 256.9 \text{ K} < T < 283.6 \text{ K} \\ \tilde{\rho}(\text{gas}) &= 0.01406 - 5.28752 \times 10^{-5}T \\ &\quad + 6.43629 \times 10^{-8}T^2 \quad T > 283.6 \text{ K} \end{aligned}$$

6.22 (22) *n*-Heptane

The reduced Gibbs free energy \tilde{G} for *n*-heptane

$$\tilde{G} = -\tilde{\rho} + 3.2230 \times 10^{-4} / \tilde{\rho} + 0.0020T((1/\tilde{\rho} - 1) \times \ln(1 - \tilde{\rho}) + 0.1045 \ln(\tilde{\rho}) - 3.8021)$$

where

$$\begin{aligned} \tilde{\rho}(\text{liquid}) &= 0.9884 + 2.91576 \times 10^{-4}T \\ &\quad - 2.3692 \times 10^{-6}T^2 \quad 182.9 \text{ K} < T < 372.8 \text{ K} \\ \tilde{\rho}(\text{gas}) &= 0.01445 - 4.28445 \times 10^{-5}T \\ &\quad + 4.09813 \times 10^{-8}T^2 \quad T > 372.8 \text{ K} \end{aligned}$$

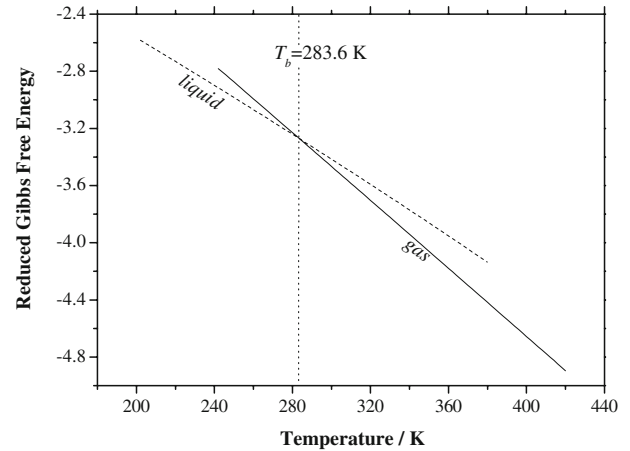


Fig. A21 Reduced Gibbs free energy of neopentane

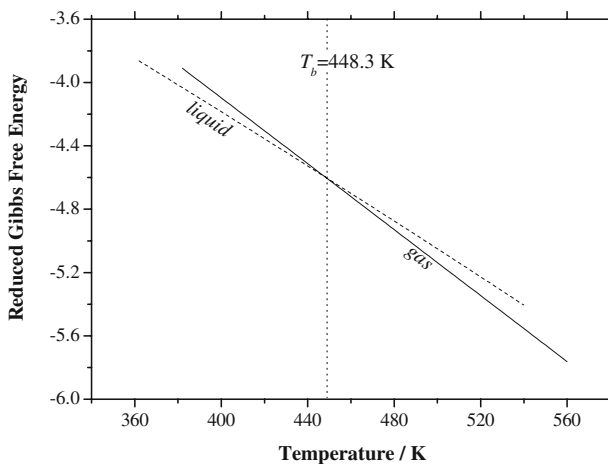


Fig. A20 Reduced Gibbs free energy of *n*-decane

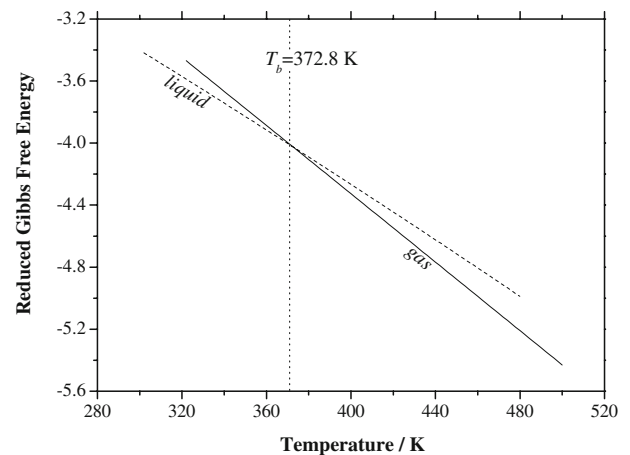


Fig. A22 Reduced Gibbs free energy of *n*-heptane

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6.23 (23) *n*-Hexane

The reduced Gibbs free energy \tilde{G} for *n*-hexane

$$\tilde{G} = -\tilde{\rho} + 3.3389 \times 10^{-4}/\tilde{\rho} + 0.0021T((1/\tilde{\rho} - 1) \times \ln(1 - \tilde{\rho}) + 0.1195 \ln(\tilde{\rho}) - 3.9069)$$

where

$$\begin{aligned} \tilde{\rho}(\text{liquid}) &= 0.98896 + 3.20688 \times 10^{-4}T \\ &\quad - 2.59846 \times 10^{-6}T^2 \quad 178.1 \text{ K} < T < 342.3 \text{ K} \\ \tilde{\rho}(\text{gas}) &= 0.01327 - 4.11598 \times 10^{-5}T \\ &\quad + 4.13735 \times 10^{-8}T^2 \quad T > 342.3 \text{ K} \end{aligned}$$

6.24 (24) *n*-Nonane

The reduced Gibbs free energy \tilde{G} for *n*-nonane

$$\tilde{G} = -\tilde{\rho} + 3.30033 \times 10^{-4}/\tilde{\rho} + 0.001934T((1/\tilde{\rho} - 1) \times \ln(1 - \tilde{\rho}) + 0.090416 \ln(\tilde{\rho}) - 3.9914)$$

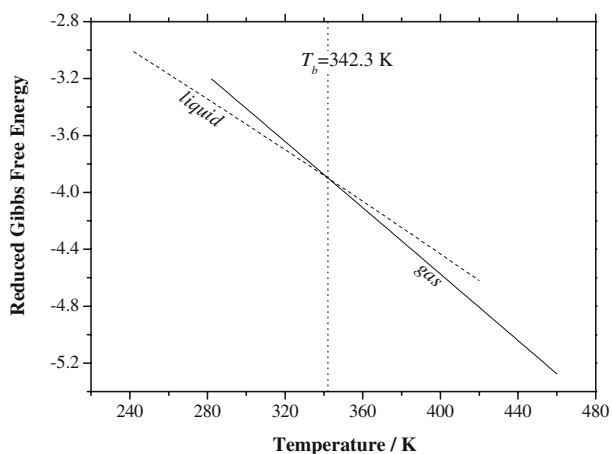


Fig. A23 Reduced Gibbs free energy of *n*-hexane

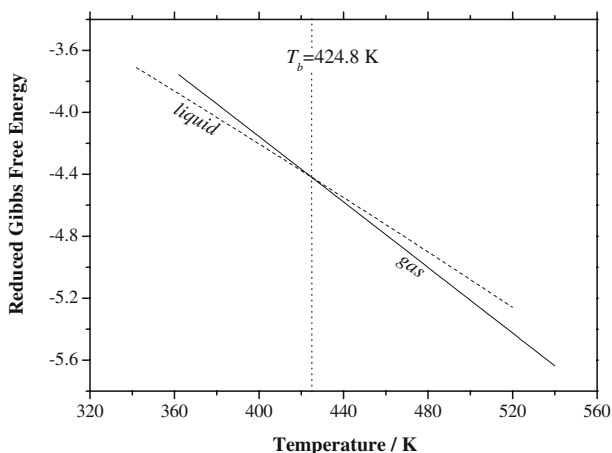


Fig. A24 Reduced Gibbs free energy of *n*-nonane

where

$$\begin{aligned} \tilde{\rho}(\text{liquid}) &= 0.98389 + 2.70838 \times 10^{-4}T \\ &\quad - 2.0142 \times 10^{-6}T^2 \quad 220 \text{ K} < T < 424.8 \text{ K} \\ \tilde{\rho}(\text{gas}) &= 0.01608 - 4.2419 \times 10^{-5}T \\ &\quad + 3.5945 \times 10^{-8}T^2 \quad T > 424.8 \text{ K} \end{aligned}$$

6.25 (25) *n*-Octane

The reduced Gibbs free energy \tilde{G} for *n*-octane

$$\tilde{G} = -\tilde{\rho} + 3.2327 \times 10^{-4}/\tilde{\rho} + 0.0020T((1/\tilde{\rho} - 1) \times \ln(1 - \tilde{\rho}) + 0.0967 \ln(\tilde{\rho}) - 3.8941)$$

where

$$\begin{aligned} \tilde{\rho}(\text{liquid}) &= 0.9822 + 3.02474 \times 10^{-4}T \\ &\quad - 2.20592 \times 10^{-6}T^2 \quad 216.7 \text{ K} < T < 399.7 \text{ K} \\ \tilde{\rho}(\text{gas}) &= 0.01504 - 4.13663 \times 10^{-5}T \\ &\quad + 3.66529 \times 10^{-8}T^2 \quad T > 399.7 \text{ K} \end{aligned}$$

6.26 (26) *n*-Pentane

The reduced Gibbs free energy \tilde{G} for *n*-pentane

$$\tilde{G} = -\tilde{\rho} + 3.2127 \times 10^{-4}/\tilde{\rho} + 0.0023T((1/\tilde{\rho} - 1) \times \ln(1 - \tilde{\rho}) + 0.1236 \ln(\tilde{\rho}) - 3.5064)$$

where

$$\begin{aligned} \tilde{\rho}(\text{liquid}) &= 0.98942 + 3.51477 \times 10^{-4}T \\ &\quad - 3.07531 \times 10^{-6}T^2 \quad 143.8 \text{ K} < T < 309.9 \text{ K} \\ \tilde{\rho}(\text{gas}) &= 0.01293 - 4.53921 \times 10^{-5}T \\ &\quad + 5.16051 \times 10^{-8}T^2 \quad T > 309.9 \text{ K} \end{aligned}$$

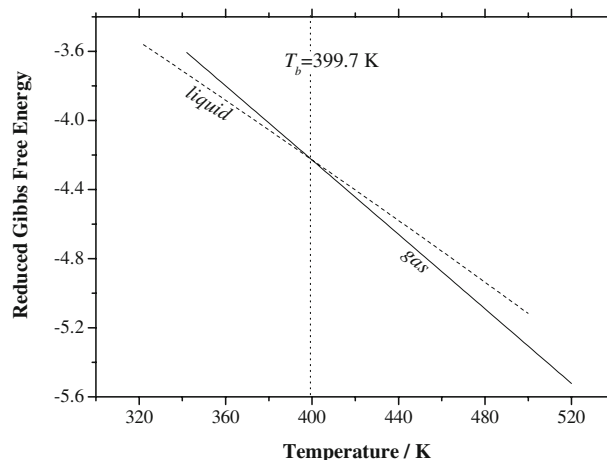


Fig. A25 Reduced Gibbs free energy of *n*-octane

6.27 (27) o-Xylene

The reduced Gibbs free energy \tilde{G} for o-xylene

$$\tilde{G} = -\tilde{\rho} + 2.5236 \times 10^{-4}/\tilde{\rho} + 0.0017T((1/\tilde{\rho} - 1) \times \ln(1 - \tilde{\rho}) + 0.1094 \ln(\tilde{\rho}) - 2.9936)$$

where

$$\begin{aligned} \tilde{\rho}(\text{liquid}) &= 0.9887 + 2.52918 \times 10^{-4}T \\ &\quad - 1.74527 \times 10^{-6}T^2 \quad 248.3 \text{ K} < T < 418.2 \text{ K} \\ \tilde{\rho}(\text{gas}) &= 0.01073 - 2.74533 \times 10^{-5}T \\ &\quad + 2.28398 \times 10^{-8}T^2 \quad T > 418.2 \text{ K} \end{aligned}$$

6.28 (28) Propane

The reduced Gibbs free energy \tilde{G} for propane

$$\tilde{G} = -\tilde{\rho} + 3.1789 \times 10^{-4}/\tilde{\rho} + 0.0027T((1/\tilde{\rho} - 1) \times \ln(1 - \tilde{\rho}) + 0.1538 \ln(\tilde{\rho}) - 3.0928)$$

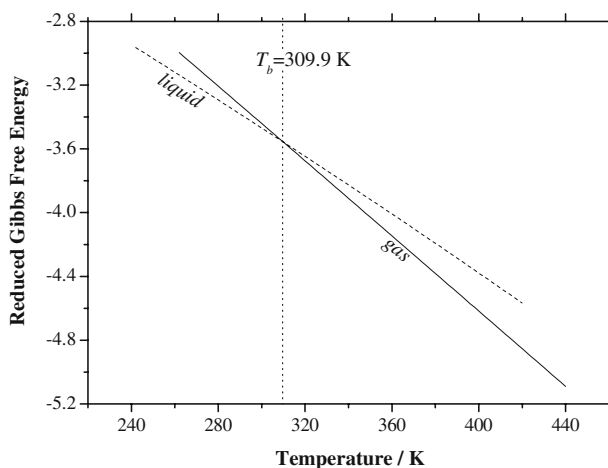


Fig. A26 Reduced Gibbs free energy of n-pentane

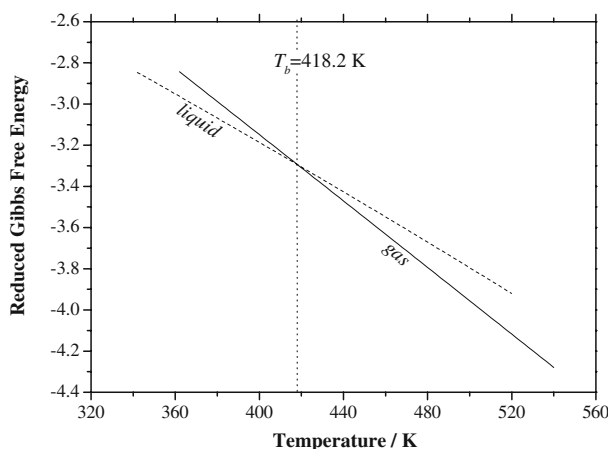


Fig. A27 Reduced Gibbs free energy of o-xylene

where

$$\begin{aligned} \tilde{\rho}(\text{liquid}) &= 0.98779 + 4.84688 \times 10^{-4}T \\ &\quad - 4.76554 \times 10^{-6}T^2 \quad 85.5 \text{ K} < T < 231.2 \text{ K} \\ \tilde{\rho}(\text{gas}) &= 0.01158 - 5.47285 \times 10^{-5}T \\ &\quad + 8.38928 \times 10^{-8}T^2 \quad T > 231.2 \text{ K} \end{aligned}$$

6.29 (29) p-Xylene

The reduced Gibbs free energy \tilde{G} for p-xylene

$$\tilde{G} = -\tilde{\rho} + 2.6137 \times 10^{-4}/\tilde{\rho} + 0.0018T((1/\tilde{\rho} - 1) \times \ln(1 - \tilde{\rho}) + 0.1094 \ln(\tilde{\rho}) - 2.997)$$

where

$$\begin{aligned} \tilde{\rho}(\text{liquid}) &= 0.98356 + 2.85265 \times 10^{-4}T \\ &\quad - 1.84572 \times 10^{-6}T^2 \quad 286.5 \text{ K} < T < 412.2 \text{ K} \\ \tilde{\rho}(\text{gas}) &= 0.01091 - 2.79056 \times 10^{-5}T \\ &\quad + 2.32129 \times 10^{-8}T^2 \quad T > 412.2 \text{ K} \end{aligned}$$

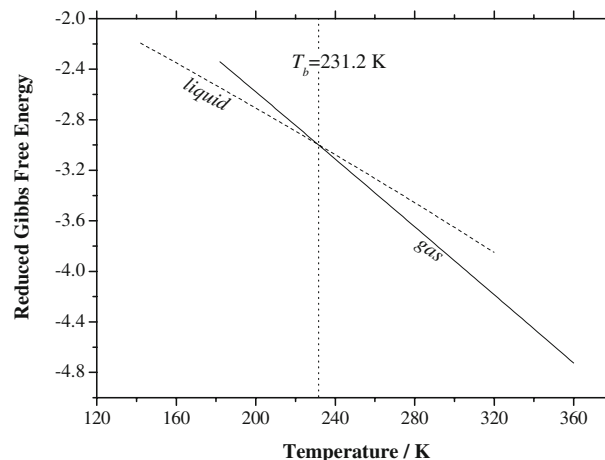


Fig. A28 Reduced Gibbs free energy of propane

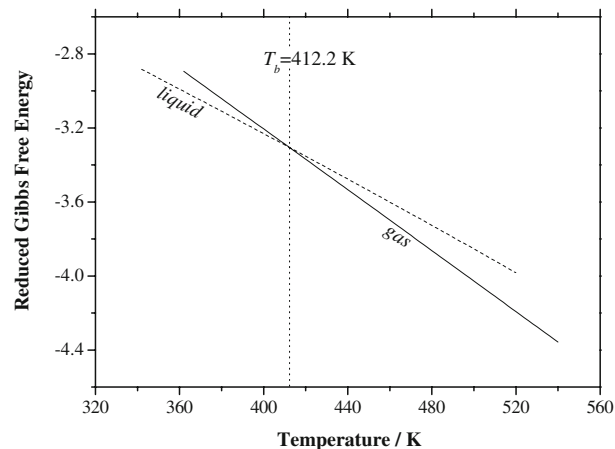


Fig. A29 Reduced Gibbs free energy of p-xylene

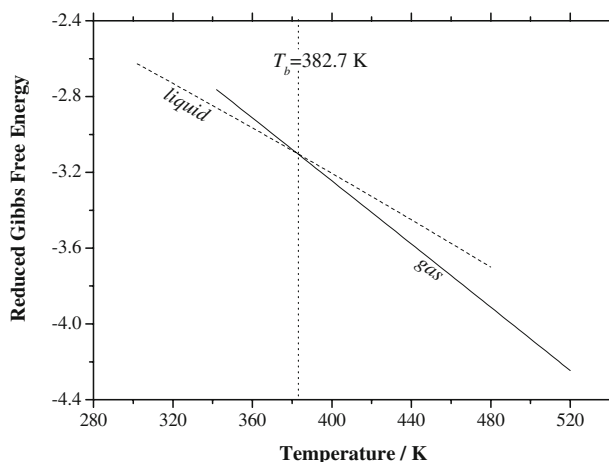


Fig. A30 Reduced Gibbs free energy of toluene

6.30 (30) Toluene

The reduced Gibbs free energy \tilde{G} for toluene

$$\tilde{G} = -\tilde{p} + 2.4735 \times 10^{-4}/\tilde{p} + 0.0018T((1/\tilde{p}) - 1) \times \ln(1 - \tilde{p}) + 0.1176 \ln(\tilde{p}) - 2.8508$$

where

$$\tilde{p}(\text{liquid}) = 0.99266 + 2.55418 \times 10^{-4}T - 1.95051 \times 10^{-6}T^2 \quad 178.6 \text{ K} < T < 382.7 \text{ K}$$

$$\tilde{p}(\text{gas}) = 0.00992 - 2.7187 \times 10^{-5}T + 2.42905 \times 10^{-8}T^2 \quad T > 382.7 \text{ K}$$

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