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Supplementary Material Available: The complete Table VI, thermodynamic properties of *n*-pentane (78 pages). Ordering information is given on any current masthead page.

PVT Surface and Thermodynamic Properties of Isopentane

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Selected values of vapor pressure, specific volume, enthalpy, and entropy are presented for the saturated liquid and vapor states of isopentane from normal boiling point (301.025 K) to the critical point (460.39 K). Experimental values of the density, together with the saturated vapor densities, were fitted to a differential regional Benedict-Webb-Rubin (DR-BWR) equation of state; compressibility factors were generated from 301 to 600 K with pressure to 300 atm. Thermodynamic properties of the real gas, $H - H^0$, $(H - H^0)/T$, $A - A^0$, $S - S^0$, $S - S^l$, $G - G^0$, $(G - G^0)/T$, $G - G^l$, and f/P, were also calculated from the classical relationships.

Previous correlation studies (*2, 6*) present both vapor–liquid coexistence and superheated vapor thermodynamic properties of isopentane. The present compilation is part of a general revision of the j-tables of the API Research Project 44 (*26*) for C_1–C_5 alkanes.

Physical Constants

Table I is a list of the physical constants and conversion factors (*34*) used in this investigation. A summary of selected, experimentally determined, critical constants is shown in Table II. The present set of critical constants (T_c = 460.39 ± 0.10 K; P_c = 33.37 ± 0.10 atm; ρ_c = 0.236 ± 0.005 g cm^{-3}) is based on the measurements of Vohra and Kobe (*31*) and Ambrose et al. (*3*). These critical constants are the same as those selected by Kudchadker et al. (*15*) and differ but slightly from those selected earlier by Kobe and Lynn (*14*).

Vapor Pressure

A Frost-Kalkwarf vapor pressure equation was used with the parameters determined to fit the experimental literature values from the normal boiling point (NBP) to the CP.

$$\log P = 22.670\,65 - 2152.74/T - 6.267\,84 \log T + 1401.44\,(P/T^2) \quad (1)$$

where P is in atm and T is in K.

† Deceased.

Table I. Physical Constants and Conversion Factors

Constants	Value
Critical temperature	460.39 K
Critical pressure	33.37 atm
Critical density	0.236 g cm^{-3}
Critical volume	306 cm^3 mol^{-1}
Normal boiling point	301.025 K
Triple point	113.25 K
Molecular weight	72.1514 mass units
Gas constant, R	82.056 06 atm cm^3 K^{-1} mol^{-1}
Temperature conversions	0 °C = 273.15 K
	0 °F = 459.67 °R
Pressure conversions	1 atm = 760 mmHg
	1 psia = 0.068 045 96 atm
Energy conversions	1 defined thermochemical calorie = 4.1840 J (exact)

Table II. Critical Constants of Isopentane

Investigator	T_c, K	P_c, atm	ρ_c, g cm^{-3}
Powlewski (*22*) (1882)	467.95	—	—
Altschul (*1*) (1893)	460.25	33.3	—
Young (*37*) (1910)	460.95	32.9	0.2343
Sugden (*29*) (1927)	—	—	0.2343
Kobe and Lynn (*14*) (1953)	460.95	32.9	0.234
Vohra and Kobe (*31*) (1959)	460.95	33.66	0.236
Ambrose, Cox, and Townsend (*3*) (1960)	460.39	—	—
Selected values (ref 15 and this work)	460.39	33.37	0.236

This equation correlates the measurements of Isaac, Li, and Canjar (*13*); Silberberg, McKetta, and Kobe (*28*); Willingham et al. (*35*); and Young (*37*) with an average deviation of 0.021 atm. In addition, the equation is in approximate agreement (average deviation of 0.04 atm) with the data of Echols and Gelus (*8*) and Schumann et al. (*24*) which were not used to determine the constants of eq 1. At the NBP of 301.025 K and the CP of 460.39

Table III. Saturated Properties of Isopentane

T, K	P, atm	dP/dT (atm K^{-1})	V_{SL}, cm^3 mol^{-1}	V_{SV}, cm^3 mol^{-1}	λ, cal mol^{-1}	H_{SL}, cal mol^{-1}	H_{SV}, cal mol^{-1}	S_{SL}, cal mol^{-1} K^{-1}	ΔS_S, cal mol^{-1} K^{-1}	S_{SV}, cal mol^{-1} K^{-1}
301.025	1.000	0.034 83	117.8	23635	5968	0	5968	0	19.82	19.82
310.0	1.351	0.043 96	119.7	17787	5827	361	6188	1.18	18.80	19.98
320.0	1.848	0.055 84	121.8	13223	5666	766	6432	2.47	17.71	20.18
330.0	2.474	0.069 62	124.1	10 014	5499	1190	6689	3.75	16.66	20.41
340.0	3.247	0.085 39	126.6	7706	5326	1595	6921	5.00	15.66	20.66
350.0	4.189	0.103 23	129.3	6014	5146	2020	7166	6.21	14.70	20.91
360.0	5.319	0.123 25	132.3	4747	4956	2453	7409	7.40	13.77	21.17
370.0	6.661	0.145 55	135.5	3783	4754	2890	7644	8.60	12.85	21.45
380.0	8.238	0.170 28	139.2	3039	4541	3347	7888	9.81	11.95	21.76
390.0	10.075	0.197 63	143.2	2454	4311	3828	8139	11.04	11.05	22.09
400.0	12.200	0.227 9	147.9	1988	4060	4361	8421	12.38	10.15	22.53
410.0	14.644	0.261 3	153.4	1611	3779	4894	8673	13.68	9.22	22.90
420.0	17.439	0.298 5	160.0	1302	3465	5447	8912	15.01	8.25	23.26
430.0	20.629	0.340 3	168.4	1041	3090	6041	9131	16.39	7.19	23.58
440.0	24.264	0.387 9	179.8	815.0	2624	6658	9182	17.82	5.96	23.78
445.0	26.269	0.414 4	187.5	708.5	2325	7015	9340	18.57	5.22	23.79
450.0	28.413	0.443 3	197.8	605.1	1962	7404	9366	19.44	4.36	23.80
451.0	28.859	0.449 4	200.4	584.7	1885	7496	9381	19.63	4.18	23.81
452.0	29.312	0.455 6	203.2	564.4	1800	7584	9384	19.81	3.98	23.79
453.0	29.769	0.461 0	206.3	544.4	1712	7668	9380	19.99	3.78	23.77
454.0	30.235	0.468 3	209.8	523.8	1616	7760	9376	20.17	3.56	23.73
455.0	30.708	0.475 0	213.8	503.7	1516	7852	9368	20.36	3.33	23.69
456.0	31.185	0.481 7	218.5	483.8	1410	7937	9347	20.56	3.09	23.65
457.0	31.670	0.488 5	224.1	464.5	1299	8017	9316	20.79	2.84	23.63
458.0	32.164	0.495 6	231.3	444.6	1171	8101	9272	21.04	2.56	23.60
459.0	32.661	0.502 7	241.5	411.5	949	8205	9154	21.31	2.07	23.38
459.5	32.915	0.506 5	249.0	391.0	800	8257	9057	21.44	1.74	23.18
460.0	33.167	0.510 1	261.1	363.6	582	8325	8907	21.65	1.27	22.92
460.39	33.370	0.512 9	306	306	0	8604	8604	22.27	0	22.27

K the equation agrees exactly with the experimental values. The equation is believed to be accurate to ±0.18% from 300 K to CP, with a maximum uncertainty of ±0.2 atm near the CP. Table III, the selected saturation properties, contains the calculated vapor pressure and its temperature derivative from the NBP to the CP.

Saturated Liquid Volume

The available measurements are those of Brown and Carr (*5*) (290–293 K); Eykman (*10*) (293 K); Grummitt et al. (*11*) (293 K); Isaac, Li, and Canjar (*13*) (398–448 K); Landolt and Jahn (*16*) (287–293 K); Maslyanskii (*18*) (293 K); Perkin (*19*) (288–298 K); Rosahov (*23*) (293 K); Timmermans (*30*) (250–288 K); Westerdijk (*32*) (293 K); Wibout et al. (*33*) (288–293 K); and Young (*37*) (273–460 K).

Selected data from the above references were fit to a modified Guggenheim (*12*) equation which was further modified as shown below to pass through the CP. The constants of the equation were evaluated for two temperature zones meeting at 313.15 K.

$$\rho_{SL} = (\rho_L + A\theta + B\theta^2)\,(1.0 + 1.0\theta + 0.25\theta^3) \qquad (2)$$

where $\theta = (1 - T/T_L)^{1/3}$, T is in K, and ρ is in g cm^{-3}. Constants for eq 2 are shown below.

	ρ_L	A	B	T_L
Less than 313.15 K	0.436 608	−222.679 08 × 10^{-3}	174.077 86 × 10^{-3}	393.15
More than 313.15 K	0.236	177.234 29 × 10^{-3}	−368.343 25 × 10^{-4}	460.39

The selected data are represented by the equation with a standard deviation of 0.000 46 g cm^{-3} from 250 to 460 K. Values from eq 2 appear in Table III.

Saturated Vapor Volume

Isaac, Li, and Canjar (*13*) (448 K); Silberberg, McKetta, and Kobe (*28*) (323–448 K); and Young (*37*) (273–460 K) measured the vapor volumes. These values together with experimental superheated vapor volumes (*13, 28, 31, 36*) were used to evaluate the constants for the differential regional Benedict-Webb-Rubin (DR-BWR) equation of state.

The selected densities and temperatures near the critical point were tested with the method proposed by Davis and Rice (*7*) and found to fit to a standard deviation of 8 × 10^{-4} the following equation:

$$(\rho_{SL} + \rho_{SV}) = 0.4733 + 0.5478(\rho_{SL} - \rho_{SV})^3 \qquad (3)$$

with ρ in g cm^{-3}.

Enthalpy of Vaporization

The enthalpies of vaporization computed from eq 4 below with eq 1 and previously selected vapor and liquid volumes appear in Table IV in comparison with the values reported by other authors (*2, 6, 37*). The measured enthalpy of vaporization 5900 cal mol^{-1} of Scott et al. (*25*) at 301.01 K agrees with the value of 5901 cal mol^{-1} which is calculated from Clapeyron equation,

$$\frac{dP}{dT} = \frac{\lambda}{T(V_{SV} - V_{SL})} \qquad (4)$$

after extrapolating orthobaric volumes and the vapor pressure derivatives to below the NBP.

Enthalpy of Saturated Liquid and Vapor

As no specific heat of saturated liquid data are available from the normal boiling point to the critical point, the saturated liquid enthalpy data reported by Arnold et al. (*2*) have been accepted

Table IV. Comparison of Enthalpies of Vaporization

	λ, cal mol^{-1}			
T, K	Y[a,b]	ALE[a,c]	DK[d]	This work
310	5760	5758	5750	5827
320	5590	5610	5575	5666
330	5425	5459	5426	5499
340	5246	5300	5280	5326
350	5086	5147	5145	5146
360	4914	4990	4959	4956
370	4729	4815	4788	4754
380	4530	4624	4590	4541
390	4302	4403	4361	4311
400	4048	4116	4090	4060
410	3776	3825	3813	3779
420	3469	3514	3471	3465
430	3100	3166	3081	3090
440	2640	2730	2603	2624
450	2030	2026	1986	1962

[a] Values are interpolated. [b] Young (*37*). [c] Arnold, Liou, and Eldridge (*2*). [d] Das and Kuloor (*6*).

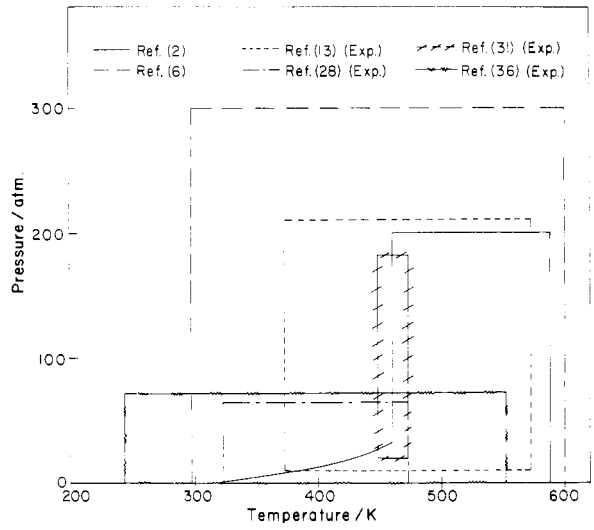

Figure 1. Regional block diagram at literature data for isopentane.

after correction for the present reference state $H_{SL} = 0$ at 301.025 K.

From the NBP to CP, the vapor enthalpy was obtained by addition of the heat of vaporization to the liquid enthalpy calculated above. The locus of $\bar{H} = (H_{SL} + H_{SV})/2$ was checked for smoothness. Values of H_{SL} and H_{SV} below 440 K indicated that the enthalpy locus was reasonably straight, and a plot of H_S vs. V_S allowed a check of the values obtained from the H_S vs. T diagram in the critical region.

Entropy of Saturated Liquid and Vapor

The saturated liquid entropy values reported by Arnold et al. (*2*) are given in Table III after correction for the present reference state $S_{SL} = 0$ at 301.025 K. The vapor entropy was obtained by the addition of (λ/T) to S_{SL}. The entropy locus, $\bar{S}_S = (S_{SL} + S_{SV})/2$, found to be reasonably straight. Again a plot of S_S vs. V_S provided a check of entropy values at densities near the critical point.

Compressibility Data

The measurements of Bridgman (*4*) covered near zero to 8711 atm with a temperature range of 273–368 K for the liquid region only. Isaac et al. (*13*) reported the values for the pressure range 10–213 atm and 373–573 K. Silberberg et al. (*28*) determined the compressibility data for 1–65 atm and 323–473 K. Vohra and Kobe (*31*) reported their data for the pressure range of 20–182 atm and 448–473 K. Young (*36*) covered 1–72.5 atm and 243–553 K. Figure 1 shows the P, T regions of these major data sources.

Correlation Procedure

Although agreement between the major data sources is not perfect, no sound reason was found for deletion of any point, and

Table V. Constants for the DR-BWR Equation: Isopentane

	Region I	Region II
No. of data points	1202	61
Density range, g mol cm^{-3}	0.000 025 6 to 0.003 315 8	0.003 315 8 to 0.006 516 31
Normalized density range	0.003 932 9 to 0.508 85	0.508 85 to 1.0
Av percentage of deviation of Z	0.457 99	0.810 54
Max percentage deviation of Z	1.924 80	3.8928
Constants for eq 5[a]		
K_{1r}	$1.195\,34 \times 10^{-2}$	$-1.010\,43 \times 10^{-1}$
K_{2r}	$-8.720\,37 \times 10^{2}$	$7.275\,91 \times 10^{3}$
K_{3r}	$-4.889\,53 \times 10^{7}$	$-7.792\,09 \times 10^{8}$
K_{4r}	$4.799\,44 \times 10^{-4}$	$5.884\,72 \times 10^{-1}$
K_{5r}	$5.652\,96 \times 10^{1}$	$-4.093\,28 \times 10^{4}$
K_{6r}	$4.585\,28 \times 10^{2}$	$2.289\,47 \times 10^{4}$
K_{7r}	$1.173\,42 \times 10^{8}$	$4.105\,54 \times 10^{9}$
K_{8r}	3.200 00	3.225 00
BWR constants[b]		
A_0	$2.053\,68 \times 10^{7}$	
B_0	$2.815\,06 \times 10^{2}$	
C_0	$1.151\,50 \times 10^{12}$	
a	$-2.043\,01 \times 10^{8}$	
b	$1.734\,54 \times 10^{3}$	
c	$4.240\,81 \times 10^{14}$	
α	$-2.931\,47 \times 10^{7}$	
γ	$7.536\,10 \times 10^{4}$	

[a] Only for use in eq 5 with ρ normalized as (g mol cm^{-3}/0.006 516 31). [b] $P - RT\rho = (B_0RT - A_0 - C_0/T^2)\rho^2 + (bRT - a)\rho^3 + a\alpha\rho^6 + (c\rho^3/T^2)[(1 + \gamma\rho^2)e^{-\gamma\rho^2}]$; P (atm), T (K), ρ (g mol cm^{-3}).

Table VI. Thermodynamic Properties of Isopentane

Pressure, atm	Z	$H - H^0$ (cal mol^{-1})	$(H - H^0)/T$ (cal mol^{-1} K^{-1})	$A - A^0$ (cal mol^{-1})	$S - S^0$ (cal mol^{-1} K^{-1})	$S - S^I$ (cal mol^{-1} K^{-1})	$G - G^0$ (cal mol^{-1})	$(G - G^0)/T$ (cal mol^{-1} K^{-1})	$G - G^I$ (cal mol^{-1})	(f/P)
					Temperature = 310 K					
1	0.9595	−80.690	−0.260	0.424	−0.1812	−0.1812	−24.5	−0.079	−24.5	0.9609
1.35[a]	0.9445	−110.482	−0.356	185.903	−0.8459	−0.2488	151.8	0.490	−33.3	0.9473
					Temperature = 330 K					
1	0.9671	−69.644	−0.211	0.289	−0.1466	−0.1466	−21.3	−0.064	−21.3	0.9681
2.47[a]	0.9149	−180.616	−0.547	595.614	−2.1832	−0.3845	539.9	1.636	−53.7	0.9213
					Temperature = 350 K					
1	0.9729	−60.858	−0.174	0.201	−0.1207	−0.1207	−18.6	−0.053	−18.6	0.9736
4	0.8832	−263.963	−0.754	967.562	−3.2868	−0.5338	886.4	2.533	−77.1	0.8950
4.19[a]	0.8771	−278.049	−0.794	1000.053	−3.4076	−0.5631	914.6	2.613	−81.0	0.8900
					Temperature = 370 K					
1	0.9775	−53.739	−0.145	0.143	−0.1009	−0.1009	−16.4	−0.044	−16.4	0.9779
4	0.9045	−229.112	−0.619	1021.318	−3.1898	−0.4369	951.1	2.571	−67.5	0.9123
6.66[a]	0.8301	−409.574	−1.107	1402.493	−4.5601	−0.7943	1277.7	3.453	−115.7	0.8543
					Temperature = 390 K					
1	0.9811	−47.878	−0.123	0.103	−0.0855	−0.0855	−14.5	−0.037	−14.5	0.9814
4	0.9207	−201.564	−0.517	1075.545	−3.1172	−0.3643	1014.2	2.600	−59.5	0.9261
8	0.8286	−439.059	−1.126	1619.993	−4.9393	−0.8098	1487.3	3.813	−123.2	0.8529
10.08[a]	0.7726	−585.382	−1.501	1806.685	−5.6820	−1.0945	1630.6	4.181	−158.5	0.8149
					Temperature = 410 K					
1	0.9840	−42.987	−0.105	0.075	−0.0732	−0.0732	−13.0	−0.032	−13.0	0.9842
4	0.9335	−179.242	−0.437	1130.047	−3.0614	−0.3084	1075.9	2.624	−52.8	0.9372
8	0.8589	−382.951	−0.934	1699.446	−4.7988	−0.6694	1584.6	3.865	−108.5	0.8752
12	0.7715	−625.673	−1.526	2041.171	−6.0507	−1.1161	1855.1	4.525	−168.1	0.8135
14.64[a]	0.7014	−823.921	−2.010	2217.970	−6.8263	−1.4963	1974.9	4.817	−210.4	0.7722
					Temperature = 430 K					
1	0.9864	−38.855	−0.090	0.055	−0.0634	−0.0634	−11.6	−0.027	−11.6	0.9865
4	0.9437	−160.815	−0.374	1184.729	−3.0175	−0.2645	1136.7	2.643	−47.1	0.9464
8	0.8822	−338.882	−0.788	1780.053	−4.6938	−0.5644	1679.5	3.906	−96.2	0.8934
12	0.8132	−541.506	−1.259	2133.540	−5.8500	−0.9154	1974.0	4.591	−147.9	0.8410
16	0.7325	−783.188	−1.821	2393.078	−6.8554	−1.3495	2164.6	5.034	−202.9	0.7885
20	0.6290	−1102.459	−2.564	2612.018	−7.9017	−1.9526	2295.3	5.338	−262.8	0.7351
20.63[a]	0.6087	−1166.698	−2.713	2645.744	−8.0891	−2.0786	2311.6	5.376	−272.9	0.7264
					Temperature = 450 K					
1	0.9883	−35.327	−0.079	0.040	−0.0554	−0.0554	−10.4	−0.023	−10.4	0.9884
4	0.9521	−145.355	−0.323	1239.523	−2.9823	−0.2293	1196.7	2.659	−42.2	0.9539
8	0.9006	−303.185	−0.674	1861.324	−4.6126	−0.4832	1772.5	3.939	−85.8	0.9085
12	0.8445	−477.434	−1.061	2228.415	−5.7043	−0.7696	2089.5	4.643	−131.1	0.8635
16	0.7822	−674.622	−1.499	2493.782	−6.6083	−1.1024	2299.1	5.109	−178.5	0.8189
20	0.7104	−906.951	−2.015	2707.222	−7.4563	−1.5073	2448.4	5.441	−228.7	0.7742
24	0.6219	−1203.182	−2.674	2895.363	−8.3570	−2.0459	2557.5	5.683	−282.5	0.7289
28	0.4875	−1684.136	−3.743	3093.114	−9.5983	−2.9810	2635.1	5.856	−342.7	0.6815
28.41[a]	0.4649	−1770.018	−3.933	3119.492	−9.8030	−3.1567	2641.3	5.870	−349.5	0.6763
					Temperature = 455 K					
1	0.9887	−34.525	−0.076	0.037	−0.0536	−0.0536	−10.1	−0.022	−10.1	0.9888
4	0.9539	−141.873	−0.312	1253.235	−2.9746	−0.2216	1211.6	2.663	−41.0	0.9556
8	0.9046	−295.289	−0.649	1881.715	−4.5951	−0.4657	1795.5	3.946	−83.4	0.9118

12	0.8512	−463.652	−1.019	2252.377	−5.6738	−0.7392	2117.9	4.655	−127.3	0.8686
16	0.7923	−652.382	−1.434	2519.667	−6.5592	−1.0532	2332.0	5.125	−173.2	0.8256
20	0.7256	−871.134	−1.915	2733.416	−7.3772	−1.4281	2485.5	5.463	−221.3	0.7827
24	0.6460	−1140.222	−2.506	2918.740	−8.2178	−1.9067	2598.9	5.712	−272.7	0.7395
28	0.5391	−1521.249	−3.343	3098.546	−9.2381	−2.6209	2682.1	5.895	−328.7	0.6950
29	0.5023	−1659.559	−3.647	3148.314	−9.5784	−2.8915	2698.6	5.931	−343.9	0.6834
30	0.4547	−1846.043	−4.057	3206.031	−10.0206	−3.2664	2713.3	5.963	−359.8	0.6715
30.71[a]	0.4024	−2063.416	−4.535	3262.344	−10.5183	−3.7178	2722.4	5.983	−371.8	0.6626
					Temperature = 470 K					
1	0.9899	−32.286	−0.069	0.030	−0.0487	−0.0487	−9.4	−0.020	−9.4	0.9900
10	0.8926	−348.447	−0.741	2152.672	−5.1083	−0.5357	2052.4	4.367	−96.7	0.9016
20	0.7641	−781.129	−1.662	2814.785	−7.1824	−1.2333	2594.6	5.520	−201.5	0.8059
30	0.5891	−1414.021	−3.009	3238.731	−9.0834	−2.3292	2855.2	6.075	−319.3	0.7103
40	0.2295	−3450.004	−7.340	3689.999	−13.6614	−6.3358	2970.8	6.321	−472.2	0.6030
50	0.2585	−3646.517	−7.759	3713.279	−14.1866	−6.4179	3021.2	6.428	−630.1	0.5091
60	0.2949	−3718.842	−7.912	3726.286	−14.4404	−6.3097	3068.1	6.528	−753.3	0.4462
80	0.3680	−3783.394	−8.050	3746.563	−14.7662	−6.0642	3156.7	6.716	−933.2	0.3679
100	0.4386	−3810.620	−8.108	3764.440	−15.0024	−5.8572	3240.5	6.895	−1057.7	0.3220
150	0.6046	−3835.833	−8.161	3805.192	−15.4723	−5.5220	3436.2	7.311	−1240.5	0.2647
200	0.7639	−3841.394	−8.173	3839.235	−15.8730	−5.3514	3618.9	7.700	−1326.3	0.2415
250	0.9224	−3828.260	−8.145	3866.323	−16.2174	−5.2526	3793.9	8.072	−1359.5	0.2330
300	1.0806	−3798.346	−8.082	3888.697	−16.5155	−5.1887	3963.9	8.434	−1359.7	0.2330
					Temperature = 500 K					
1	0.9919	−28.447	−0.057	0.018	−0.0408	−0.0408	−8.0	−0.016	−8.0	0.9919
10	0.9152	−301.116	−0.602	2288.382	−5.0105	−0.4380	2204.2	4.408	−82.1	0.9206
20	0.8200	−650.291	−1.301	2984.403	−6.9120	−0.9630	2805.7	5.611	−168.8	0.8437
30	0.7097	−1076.906	−2.154	3404.010	−8.3853	−1.6311	3115.8	6.232	−261.4	0.7686
40	0.5771	−1642.563	−3.285	3720.970	−9.8872	−2.5617	3301.0	6.602	−361.7	0.6947
50	0.4363	−2398.162	−4.796	3973.146	−11.6232	−3.8545	3413.4	6.827	−470.9	0.6224
60	0.3671	−3034.572	−6.069	4113.313	−13.0389	−4.9082	3484.9	6.970	−580.5	0.5573
80	0.3932	−3462.930	−6.926	4193.636	−14.1081	−5.4061	3591.1	7.182	−759.9	0.4652
100	0.4532	−3588.083	−7.176	4227.422	−14.5452	−5.4000	3684.5	7.369	−888.1	0.4089
150	0.6106	−3696.294	−7.393	4283.174	−15.1857	−5.2354	3896.6	7.793	−1078.6	0.3375
200	0.7651	−3727.863	−7.456	4325.299	−15.6399	−5.1182	4092.1	8.184	−1168.7	0.3082
250	0.9175	−3730.257	−7.461	4359.790	−16.0162	−5.0515	4277.9	8.556	−1204.5	0.2973
300	1.0688	−3713.617	−7.427	4388.938	−16.3417	−5.0149	4457.3	8.914	−1206.2	0.2968
					Temperature = 600 K					
1	0.9959	−19.713	−0.033	0.003	−0.0248	−0.0248	−4.9	−0.008	−4.9	0.9959
10	0.9588	−201.478	−0.336	2743.782	−4.8270	−0.2545	2694.7	4.491	−48.8	0.9599
20	0.9170	−413.080	−0.688	3570.291	−6.4741	−0.5251	3471.4	5.786	−98.0	0.9210
30	0.8747	−635.266	−1.059	4054.124	−7.5669	−0.8127	3904.9	6.508	−147.7	0.8834
40	0.8327	−867.752	−1.446	4397.166	−8.4427	−1.1171	4197.9	6.996	−197.5	0.8473
50	0.7919	−1108.760	−1.848	4661.904	−9.2046	−1.4359	4414.0	7.357	−247.2	0.8126
60	0.7539	−1354.111	−2.257	4875.155	−9.8934	−1.7627	4582.0	7.637	−296.5	0.7797
80	0.6937	−1828.248	−3.047	5194.756	−11.0968	−2.3948	4829.8	8.050	−391.4	0.7200
100	0.6625	−2228.803	−3.715	5411.767	−12.0640	−2.9189	5009.6	8.349	−477.5	0.6698
150	0.6996	−2772.926	−4.622	5690.911	−13.5099	−3.5596	5333.0	8.888	−637.2	0.5858
200	0.8059	−2970.685	−4.951	5820.481	−14.2665	−3.7449	5589.2	9.315	−723.8	0.5447
250	0.9309	−3044.482	−5.074	5901.632	−14.7730	−3.8082	5819.3	9.699	−759.6	0.5286
300	1.0606	−3066.731	−5.111	5962.899	−15.1698	−3.8430	6035.2	10.059	−760.9	0.5280

[a]Saturation pressure.

Table VII. Compressibility Factors from Corresponding States

		Z					
T, K	P, atm	ALE[a,b]	DK[a,c]	ILC[a,d]	Pitzer[e]	LGH[f]	This work
450	10	0.8775	0.8756	—	0.877	0.88	0.8737
	20	0.7189	0.7152	—	0.717	0.71	0.7104
500	80	0.3862	0.3974	0.3894	0.391	0.38	0.3932
	100	0.4376	0.4531	0.4868	0.460	0.45	0.4532
	200	0.7050	0.7683	0.7896	0.756	0.77	0.7651
550	80	0.5113	0.5538	0.5317	0.542	0.52	0.5410
	100	0.5086	0.5548	0.5646	0.580	0.55	0.5390
	200	0.6986	0.7866	0.7999	0.772	0.76	0.7784

[a] Values are interpolated. [b] Arnold, Liou, and Eldridge (*2*). [c] Das and Kuloor (*6*). [d] Isaac, Li, and Canjar (*13*). [e] Pitzer (*20*); Pitzer et al. (*21*). [f] Lydersen et al. (*17*).

each was given equal weight. Saturated vapor volumes selected in Table III were added to the present PVT data sets and given a weight of four, except for the CP and the NBP which were each weighted ten. This procedure was used to force the fitted PVT surface to values consistent with the selected saturated properties which form a boundary condition. The differential regional BWR equation is (*9*):

$$\phi = \sum_{r=1}^{N} \sum_{j=1}^{7} K_{jr}\theta_j^* \tag{5}$$

where $\phi = P - RT\rho$, $\theta_1^* = RT(\rho^*)^2$, $\theta_2^* = (\rho^*)^2$, $\theta_3^* = (\rho^*)^2T^{-2}$, $\theta_4^* = RT(\rho^*)^3$, $\theta_5^* = (\rho^*)^3$, $\theta_6^* = (\rho^*)^6$, $\theta_7^* = (\rho^*)^3[1 + K_{8r}(\rho^*)^2][\exp(-K_{8r}\rho^*)^2]T^{-2}$, $\rho^* = \rho - \rho_{r-1,n_{r-1}}$, with $\rho_{r-1,n_{r-1}}$ equal to the density at the interface between regions r and $r-1$ when the density falls in region r.

Anomalies were observed in preliminary fits at the regional interface. This was caused by lack of constraint on the region I fitting surface by data beyond the interface and could not be corrected by the region II equation. This problem was solved by an overlap fitting technique in which about 10% of the points in the next higher region adjacent to the interface were included in the fit of the region. The interface between the first and second regions was chosen to be critical density. For *n*-pentane there were not sufficient data at densities above the critical to require more than one region. Standard BWR coefficients for the first region ($K_{11} = B_0$, $K_{21} = -A_0$, $K_{31} = -C_0$, $K_{41} = b$, $K_{51} = -a$, $K_{61} = a\alpha$, $K_{71} = c$, and $K_{81} = +\gamma$) and coefficients of eq 5 for the first and second regions are found in Table V. The latter coefficients are used only with normalized densities. Table V also provides the first region constants in the usual metric units for comparison to literature BWR coefficients.

Accuracy of Saturated Properties

The selected liquid volumes of Table III are considered accurate to a maximum of ±0.3% from the NBP to 360 K, 0.4% from 360 to 440 K, and 0.2% from 440 to 460 K. The error limits of vapor volume at the NBP are ±23 cm^3 mol^{-1}, providing the measurement of enthalpy of vaporization of Scott et al. (*25*) is correct. The accuracy of enthalpy of vaporization values in Table III depends on that of the vapor pressure slope and the vapor volume with error limits of 1.4% for dP/dT.

PVT Surface and Corresponding Thermodynamic Properties

Table V shows the ability of the DR-BWR model to fit the available experimental PVT data. Both experimental data and isotherms from the model were plotted as compressibility factor $Z = (P/\rho RT)$ vs. pressure on large graphs such that the finest division was 0.0005 for Z. The Z–P graphs show that in all regions the model provides a smooth surface with reasonable compromise between the experimental results.

Table VIII. Second Virial Coefficient

	−B, cm^3 mol^{-1}		
T, K	Ref 27	Ref 28	This work
273.15	1370.6	—	1323
298.15	1149.7	—	1087
323.15	954.0	960	909
348.15	775.2	763	770
373.15	642.9	645	659
398.15	555.7	570	569
423.15	482.5	494	495
448.15	419.1	434	433
461.65	388.4	407	403
473.15	366.4	376	380

Thermodynamic properties were calculated from the PVT surface by the usual relationships and appear in Table VI, a condensed version of the API Research Project 44 j-tables (a complete version of Table VI has been deposited in the ACS Microfilm Depository Service). Values of pressure in parentheses are at saturated conditions. The tables are thermodynamically consistent as the other functions were calculated from $A - A^0$ and $S - S^0$, where A is the energy function for density and temperature with S its temperature derivative. Table VI extends only to 600 K or slightly above the maximum experimental temperature of 573 K rather than 1500 K as in the revised API Research Project 44 Tables. The values above 573 K are an extrapolation of the present surface and further assume no decomposition of isopentane.

Discussion

Table VII is a comparison of present values with those calculated from corresponding states by two methods: The corresponding state tables of Lydersen et al. (*17*) and Pitzer's (*20, 21*), acentric factor procedure. Table VIII is a comparison of the selected second virial coefficients of Silberberg et al. (*27, 28*) with the present values where:

$$B = B_0 - \frac{A_0}{RT} - \frac{C_0}{RT^3} \tag{6}$$

The present PVT surface was not constrained by the critical conditions:

$$\left(\frac{\partial P}{\partial \rho}\right)_{T_c} = 0 = \left(\frac{\partial^2 P}{\partial \rho^2}\right)_{T_c} \tag{7}$$

However, the constants of Table V for the region yield $(\partial P_r/\partial \rho_r)_{T_r=1} = 0.0288$ and $(\partial^2 P_r/\partial \rho_r{}^2)_{T_r=1} = 0.4225$.

Glossary

A	Helmholtz energy, cal mol^{-1}
$A_0,B_0,C_0,$ a,b,c,α,γ	BWR constants in atm cm^3 K^{-1} mol^{-1} units
B	second virial coefficient, cm^3 mol^{-1}
CP	critical point, 460.39 K
f	fugacity, atm
G	Gibbs energy, cal mol^{-1}
H	enthalpy, cal mol^{-1}
K	constants of eq 5
N	total number of regions
NBP	normal boiling point, 301.025 K
n	number of data points in a given region
P	pressure, atm
R	gas constant, 82.056 06 atm cm^3 K^{-1} mol^{-1}
S	entropy, cal K^{-1} mol^{-1}
T	temperature, K
V	specific volume, cm^3 mol^{-1}
Z	compressibility factor

Greek Letters

λ	latent heat of vaporization, cal mol^{-1}
θ	dimensionless temperature variable defined by eq 2
θ^*	density and temperature-dependent factors defined in eq 5
ρ	density, mol cm^3
ρ_L	limiting density constant in eq 2
ϕ	$P - RT\rho$, atm

Superscripts

I	ideal gas state
0	standard state; ideal gas at 1 atm and temperature T
*	indicates difference between quantity in region i and the value of that quantity at the region $i-1$/region i interface

Subscripts

c	critical point value
i	running index for BWR terms
r	divided by critical value
r	region
S	saturated property
SV	saturated vapor
SL	saturated liquid
T_L	limiting temperature constant in eq 2

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Supplementary Material Available: The complete Table VI, thermodynamic properties of isopentane (75 pages). Ordering information is given on any current masthead page.