Solid & Liquid Heat Capacity Data Collection C1-C32 Compounds Part 2: C3-C32

Solid and Liquid Heat Capacity Data Collection

$C_1 - C_{33}$ Compounds

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Solid and liquid heat capacity data collection : $C_1 - C_{33}$

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Editor's Introduction

Since its foundation in 1926, DECHEMA has attempted to further the work of technologists and engineers by supplying them with the tools needed for their work. Nowadays software tools play an ever-increasing role in design, construction and operation of chemical plant. Modern optimisation methods have reached heights of sophistication that would have been unimaginable to engineers trained at the time of the founding of the DECHEMA. Such software needs to be built on a firm foundation of accurate data. Even the most modern software produces less than optimal solutions if the input data is not of the highest quality. With this in mind, the DECHEMA is pleased to publish the results of a long term project of collecting, collating, calculating and assessing heat capacity data for both solid and liquid states from the scientific literature. This work was carried out by a group of scientists from the Industrial Chemistry Research Institute, Warsaw. It is hoped that this data will be assistance to all those working in the fields of chemical plant modelling and optimisation.

Gerhard Kreysa

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C_6H_7N BENZENAMINE

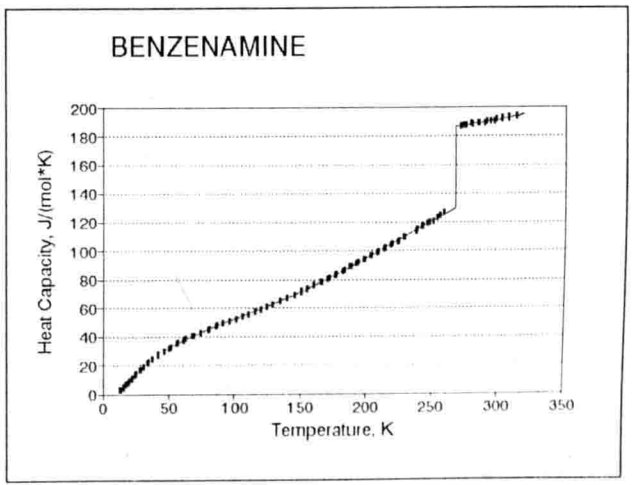
CAS REG.NO. 62-53-3

Hatton,W.E.;et al.,J.Chem.Eng.Data, 1962,7,229.

MOLAR HEAT CAPACITY OF SOLID

$(Cp)_s = -4.2381 + 1.014031*T - 0.739546*10^{-2}*T^2 + 0.346175*10^{-4}*T^3 - 0.528564*10^{-7}*T^4$

T, K	CE,J/MOL*K	CC,J/MOL*K	DEV,J/MOL*K
13.490	3.335		
13.670	3.460		
15.490	4.682		
15.790	4.833		
17.510	6.351		
17.830	6.657		
19.570	8.247		
20.210	8.858		
21.970	10.418		
22.820	11.339		
24.960	13.113		
25.660	13.690		
28.140	16.292		
28.590	16.581		
31.160	18.648		
31.540	18.928		
34.380	21.497		
34.730	21.686		
35.140	21.953		
37.940	24.167		
38.210	24.301		
38.260	24.250		
42.140	26.962		
42.190	27.204		
46.490	30.029	30.152	0.123



46.550	29.878	30.183	0.305
49.970	31.765	31.956	0.191
51.370	32.794	32.662	-0.133
56.150	35.183	34.986	-0.197
56.780	35.656	35.283	-0.373
61.350	37.476	37.382	-0.094
62.750	38.493	38.006	-0.487
67.510	40.267	40.067	-0.200
68.760	40.564	40.594	0.030
73.860	42.509	42.689	0.180
74.370	42.886	42.894	0.008
79.800	45.020	45.035	0.015
80.340	45.145	45.244	0.099
85.400	47.321	47.173	-0.148
86.850	47.781	47.718	-0.063
90.750	49.246	49.167	-0.079
95.890	50.919	51.050	0.131
100.860	52.426	52.854	0.428
105.690	54.225	54.599	0.374
110.370	55.982	56.292	0.310
114.930	57.614	57.949	0.336
119.370	59.455	59.577	0.123
123.710	60.919	61.187	0.268
128.640	62.718	63.043	0.325
134.150	65.145	65.159	0.014
139.510	67.195	67.265	0.070
144.750	69.580	69.376	-0.204
149.880	71.714	71.494	-0.220
150.090	71.881	71.582	-0.299
154.850	73.471	73.599	0.128
154.900	73.806	73.621	-0.185
159.770	75.814	75.735	-0.079
159.820	75.898	75.757	-0.140

MOLAR HEAT CAPACITY OF SOLID

$(Cp)_s = -4.2381 + 1.014031*T - 0.739546*10^{-2}*T^2 + 0.346175*10^{-4}*T^3 - 0.528564*10^{-7}*T^4$

T, K	CE,J/MOL*K	CC,J/MOL*K	DEV,J/MOL*K
164.610	78.032	77.889	-0.143
165.220	78.492	78.164	-0.328
169.890	80.500	80.297	-0.203
171.100	81.253	80.858	-0.395
175.650	83.471	82.994	-0.477
176.850	83.847	83.565	-0.282
181.290	85.939	85.703	-0.236
182.480	86.567	86.283	-0.284
186.810	88.910	88.416	-0.494
187.980	89.161	88.999	-0.162
192.220	91.295	91.131	-0.164
193.380	91.922	91.719	-0.203
197.530	93.973	93.843	-0.129
198.680	94.391	94.437	0.046
202.740	96.399	96.546	0.146
203.870	96.985	97.137	0.151
207.860	98.784	99.234	0.450
208.980	99.537	99.826	0.289
212.890	101.629	101.901	0.271
214.000	102.173	102.492	0.318
217.830	104.056	104.536	0.480
218.930	104.935	105.124	0.190
222.700	106.608	107.143	0.534
223.780	107.152	107.721	0.569
227.480	109.495	109.701	0.206
228.550	109.956	110.273	0.318
236.780	114.098	114.647	0.549
237.840	115.018	115.205	0.187
241.340	117.403	117.039	-0.364
242.390	117.612	117.586	-0.027

245.840	119.328	119.367	0.040
247.320	119.704	120.124	0.420
250.280	121.169	121.623	0.455
252.630	123.010	122.798	-0.212
255.040	124.934	123.986	-0.948
257.830	126.566	125.340	-1.226

MOLAR HEAT CAPACITY OF LIQUID

$(Cp)_l = 86.2177 + 0.290671*T + 1.642544*10^6 *T^{-2}$

T, K	CE,J/MOL*K	CC,J/MOL*K	DEV,J/MOL*K
270.220	187.192	187.258	0.066
272.590	187.611	187.557	-0.053
274.850	187.694	187.852	0.158
278.440	188.949	188.338	-0.611
279.460	188.531	188.481	-0.050
284.050	188.657	189.141	0.484
284.270	189.326	189.173	-0.153
288.630	189.410	189.831	0.421
290.090	189.954	190.057	0.104
293.190	190.414	190.548	0.134
295.880	190.790	190.984	0.193
297.720	191.878	191.287	-0.591
301.630	191.920	191.947	0.027
302.240	192.255	192.051	-0.204
306.730	193.133	192.834	-0.300
307.360	192.882	192.945	0.063
313.060	193.677	193.975	0.297

DELTA CP @ MELTING POINT(= 267.13 K) = 57.24 J/(MOL*K)
ENTHALPY OF MELTING = 10539.50 J/MOL
ENTROPY OF MELTING = 4.75

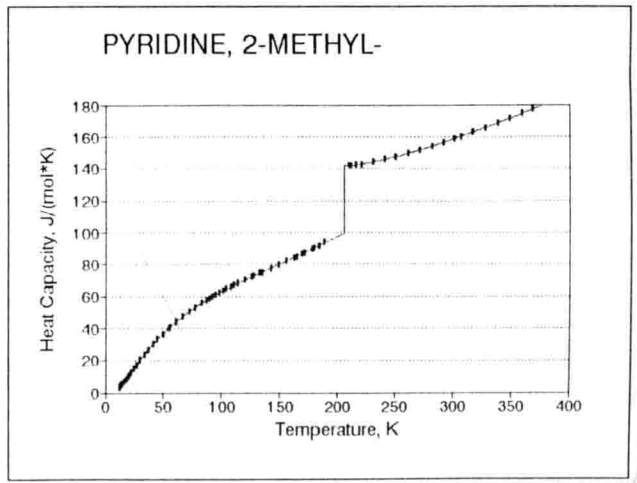
C_6H_7N PYRIDINE, 2-METHYL- CAS REG.NO. 109-06-8

Scott,D.W.;et al.,J.Phys.Chem.,1963,67,680.

MOLAR HEAT CAPACITY OF SOLID

$(Cp)_s = -17.1682 + 1.536676*T - 0.111527*10^{-1}*T^2 + 0.445126*10^{-4}*T^3 - 0.643175*10^{-7}*T^4$

T, K	CE,J/MOL*K	CC,J/MOL*K	DEV,J/MOL*K
12.370	3.389		
12.650	3.653		
13.780	4.477		
14.040	4.736		
15.200	5.636		
15.400	5.832		
16.520	6.774		
16.970	7.205		
18.110	8.251		
18.870	8.970		
20.100	10.142		
20.840	10.845		
22.240	12.251		
22.850	12.849		
24.560	14.615		
24.940	14.995		
27.240	17.288	17.280	-0.009
27.260	17.292	17.300	0.008
29.890	19.912	19.936	0.025
30.380	20.397	20.416	0.019
33.640	23.527	23.517	-0.010
37.200	26.790	26.731	-0.059
41.160	30.158	30.106	-0.052
45.290	33.422	33.416	-0.006
49.890	36.857	36.866	0.009



54.970	40.384	40.409	0.025
55.510	40.752	40.770	0.018
60.430	43.945	43.931	-0.014
60.920	44.263	44.234	-0.029
66.380	47.488	47.465	-0.024
72.020	50.430	50.553	0.123
77.840	53.350	53.504	0.154
83.730	56.312	56.277	-0.035
86.950	57.861	57.713	-0.148
89.680	58.990	58.890	-0.101
92.760	59.844	60.177	0.333
95.380	61.283	61.240	-0.043
98.350	62.396	62.414	0.018
101.410	63.559	63.591	0.032
104.280	64.680	64.669	-0.012
107.770	65.977	65.947	-0.031
110.540	66.965	66.940	-0.025
113.910	68.153	68.125	-0.028
119.890	70.228	70.177	-0.051
126.180	72.387	72.283	-0.105
127.540	72.797	72.733	-0.065
132.780	74.534	74.454	-0.080
134.910	75.199	75.150	-0.049
142.070	77.454	77.481	0.026
149.050	79.806	79.755	-0.050
155.850	82.011	81.988	-0.023
162.490	84.140	84.193	0.053
165.220	85.031	85.108	0.077
168.990	86.282	86.382	0.099
171.770	87.211	87.328	0.116
171.770	87.257	87.328	0.070
178.210	89.416	89.543	0.127
180.250	90.291	90.252	-0.039

MOLAR HEAT CAPACITY OF SOLID

$(Cp)_s = -17.1682 + 1.536676*T - 0.111527*10^{-1}*T^2 + 0.445126*10^{-4}*T^3 - 0.643175*10^{-7}*T^4$

T, K	CE,J/MOL*K	CC,J/MOL*K	DEV,J/MOL*K
184.520	91.713	91.745	0.031
188.560	93.450	93.169	-0.281

MOLAR HEAT CAPACITY OF LIQUID

$(Cp)_l = 266.9578 - 1.736759*T + 0.801448*10^{-2}*T^2 - 0.143662*10^{-4}*T^3 + 0.982302*10^{-8}*T^4$

T, K	CE,J/MOL*K	CC,J/MOL*K	DEV,J/MOL*K
209.900	141.758	141.727	-0.032
211.970	141.884	141.924	0.040
215.520	142.327	142.293	-0.034
221.090	142.921	142.946	0.025
231.030	144.294	144.319	0.025
240.870	145.942	145.912	-0.031
250.590	147.670	147.686	0.015
260.640	149.687	149.702	0.015
270.980	151.967	151.941	-0.026
281.190	154.318	154.292	-0.026
291.240	156.716	156.720	0.004
301.160	159.205	159.208	0.003
306.240	160.511	160.512	0.001
317.130	163.356	163.365	0.009
327.840	166.209	166.235	0.025
338.370	169.088	169.106	0.018
348.750	171.916	171.975	0.058
358.950	175.008	174.826	-0.182
369.010	177.577	177.667	0.090

DELTA CP @ MELTING POINT(= 206.45 K) = 41.86 J/(MOL*K)
ENTHALPY OF MELTING = 9724.00 J/MOL
ENTROPY OF MELTING = 5.66

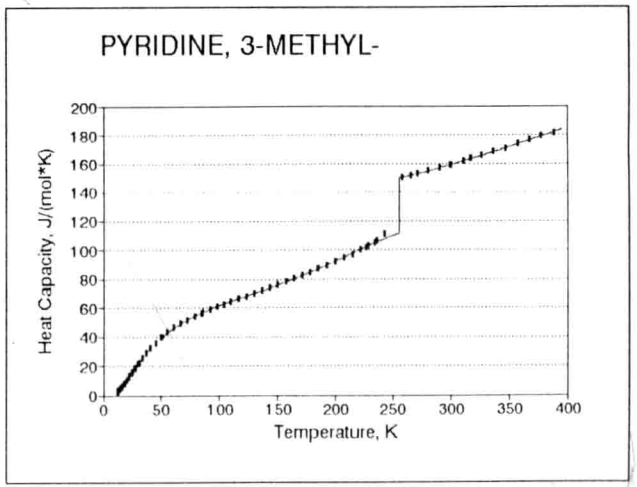
C_6H_7N PYRIDINE, 3-METHYL- CAS REG.NO. 108-99-6

Scott,D.W.;et al.,J.Phys.Chem.,1963,67,685.

MOLAR HEAT CAPACITY OF SOLID

$(Cp)_s = -12.5197 + 1.552821*T - 0.125911*10^{-1}*T^2 + 0.526736*10^{-4}*T^3 - 0.772527*10^{-7}*T^4$

T, K	CE,J/MOL*K	CC,J/MOL*K	DEV,J/MOL*K
11.940	2.473		
12.430	2.749		
13.350	3.381		
13.700	3.665		
14.790	4.506		
15.220	4.920		
16.520	6.104		
17.000	6.535		
18.550	8.092		
18.920	8.443		
20.560	10.222		
20.780	10.581		
22.530	12.418		
22.890	12.832		
24.730	14.958		
25.400	15.757		
27.290	17.937		
28.130	18.887		
30.200	21.234		
31.060	22.196		
34.100	25.522		
37.250	28.769		
40.980	32.288		
45.580	36.158		
50.130	39.643	39.829	0.186



50.570	39.953	40.114	0.161
55.450	43.229	43.121	-0.109
61.150	46.631	46.317	-0.313
66.780	49.497	49.177	-0.319
72.700	52.007	51.904	-0.103
78.950	54.538	54.514	-0.025
85.190	56.873	56.884	0.011
85.770	57.174	57.094	-0.080
91.810	59.099	59.188	0.089
98.070	60.936	61.204	0.269
104.270	62.752	63.081	0.330
110.000	64.434	64.737	0.303
116.500	66.321	66.550	0.230
123.150	68.233	68.364	0.131
130.000	70.208	70.218	0.010
136.670	72.124	72.033	-0.091
143.460	74.099	73.912	-0.187
150.380	76.115	75.878	-0.237
157.150	78.149	77.865	-0.284
164.180	80.324	80.005	-0.319
171.440	82.580	82.304	-0.275
178.540	84.847	84.642	-0.206
185.480	87.061	87.008	-0.052
192.640	89.420	89.527	0.107
199.990	91.977	92.182	0.205
207.180	94.554	94.828	0.274
214.510	97.019	97.552	0.534
221.710	99.784	100.225	0.441
226.840	101.859	102.110	0.250
228.770	102.621	102.811	0.190
234.580	105.382	104.889	-0.493
235.680	105.935	105.275	-0.659
242.350	111.131		

MOLAR HEAT CAPACITY OF LIQUID

$(Cp)_l = 292.6452 - 1.925786*T + 0.844616*10^{-2}*T^2 - 0.145356*10^{-4}*T^3 + 0.945010*10^{-8}*T^4$

T, K	CE,J/MOL*K	CC,J/MOL*K	DEV,J/MOL*K
257.520	150.164	150.161	-0.002
264.800	151.511	151.507	-0.004
271.360	152.791	152.800	0.009
280.040	154.616	154.614	-0.002
289.850	156.779	156.786	0.007
299.520	159.046	159.035	-0.011
300.240	159.201	159.207	0.005
310.420	161.640	161.676	0.035
316.650	163.285	163.226	-0.059
326.200	165.645	165.651	0.006
336.520	168.335	168.323	-0.012
347.120	171.084	171.110	0.026
357.570	173.841	173.889	0.048
367.850	176.682	176.645	-0.037
377.970	179.410	179.375	-0.035
387.930	182.050	182.075	0.025

DELTA CP @ MELTING POINT(= 255.01 K) = 38.25 J/(MOL*K)
ENTHALPY OF MELTING = 14180.40 J/MOL
ENTROPY OF MELTING = 6.69