

Gas phase constant pressure heat capacities ($C_{p,gas}$) for the C_1 through C_{10} straight chain alkanes, isobutane, hydrogen atom, hydroxyl and methyl radicals, and water between 298.15 and 1500 K: A comparison of theoretical values against experimental data

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Gas phase constant pressure heat capacities ($C_{p,gas}$) for the C_1 through C_{10} straight chain alkanes, isobutane, hydrogen atom, hydroxyl and methyl radicals, and water were calculated between 298.15 and 1500 K using various low (semiempirical PM6) through high level (CBS-Q//B3 and G4 composite) theoretical methods. All levels of theory provided good agreement with experimental $C_{p,gas}$ data ($< \pm 10\%$ deviation) regardless of molecular size. A modest but progressive loss of $C_{p,gas}$ predictive accuracy occurs with increasing molecular size among the n-alkanes. For most compounds at all levels of theory, the highest $C_{p,gas}$ estimation accuracy occurs at elevated temperatures, with decreasing accuracy as the temperature is lowered or raised about the method specific accuracy maximum. In general, $C_{p,gas}$ prediction accuracy appears to depend less on the level of theory applied compared to the temperature under consideration.

The temperature dependence of enthalpy at constant pressure (heat capacity; $C_p = (\frac{\partial H}{\partial T})_P$; H=enthalpy, T=temperature; P=pressure) plays a key role in modeling chemical processes under non-standard state conditions, such as combustion thermodynamics, astrochemistry, and biomedical science. In the current work, we calculated the gas phase C_p ($C_{p,gas}$) at 1 atmosphere pressure over a temperature range from 298.15 to 1500 K for the following various benchmark compounds relevant to combustion modeling using Gaussian 09 [1]: hydrogen atom (Table 1); methyl radical (Table 2); water (Table 3); hydroxyl radical (Table 4); methane (Table 5); ethane (Table 6); propane (Table 7); n-butane (Table 8); isobu-

tane (Table 9); n-pentane (Table 10); n-hexane (Table 11); n-heptane (Table 12); n-octane (Table 13); n-nonane (Table 14); and n-decane (Table 15). Depending on the compound under consideration, calculations were conducted at the semiempirical PM6 [2], M062X/6-311++G(d,p) density functional [3] [4] [5] [6] [7] [8], and CBS-Q//B3 [9] [10] and G4 [11] composite method levels of theory.

In general, all levels of theory provided good agreement with experimental $C_{p,gas}$ data ($< \pm 10\%$ deviation) - regardless of molecular size - for the compounds under consideration. Several trends are evident in the accuracy of the theoretical data. A modest but progressive loss of $C_{p,gas}$ predictive accuracy occurs with increasing molecular size among the n-alkanes. For most compounds at all levels of theory, the highest $C_{p,gas}$ estimation accuracy occurs at elevated temperatures (PM6: ≈ 500 K; CBS-QB3: ≈ 800 K; and G4: ≈ 900 -1000 K), with the loss of accuracy typically increasing more rapidly as the temperature is progressively lowered below this accuracy maximum compared to corresponding temperature increases above the $C_{p,gas}$ accuracy maximum. $C_{p,gas}$ prediction accuracy appears to depend less on the level of theory applied compared to the temperature under consideration.

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Table 1: Experimental and G4 calculated gas phase constant pressure heat capacities ($C_{p,gas}$) at 1 atmosphere for the hydrogen atom between 298.15 and 1500 K. Values in brackets represent percent deviations from experimental data.

T (K)	expt. [12] $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	G4 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)
298.15	4.97	4.97 [0.0%]
300	4.97	4.97 [0.0%]
500	4.97	4.97 [0.0%]
700	4.97	4.97 [0.0%]
900	4.97	4.97 [0.0%]
1100	4.97	4.97 [0.0%]
1300	4.97	4.97 [0.0%]
1500	4.97	4.97 [0.0%]

Table 2: Experimental and G4 calculated gas phase constant pressure heat capacities ($C_{p,gas}$) at 1 atmosphere for the methyl radical between 298.15 and 1500 K. Values in brackets represent percent deviations from experimental data.

T (K)	expt. [12] $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	G4 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)
298.15	9.24	9.47 [2.4%]
300	9.26	9.48 [2.4%]
500	10.81	10.88 [0.7%]
700	12.23	12.19 [-0.3%]
900	13.51	13.40 [-0.8%]
1100	14.62	14.48 [-1.0%]
1300	15.55	15.39 [-1.0%]
1500	16.29	16.14 [-0.9%]

Table 3: Experimental and G4 calculated gas phase constant pressure heat capacities ($C_{p,gas}$) at 1 atmosphere for water between 298.15 and 1500 K. Values in brackets represent percent deviations from experimental data.

T (K)	expt. [12] $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	G4 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)
298.15	7.81	7.98 [2.2%]
300	7.81	7.99 [2.3%]
500	8.42	8.34 [-1.0%]
700	8.96	8.84 [-1.3%]
900	9.56	9.40 [-1.7%]
1100	10.16	9.96 [-2.0%]
1300	10.74	10.50 [-2.3%]
1500	11.26	10.97 [-2.5%]

Table 4: Experimental and PM6, M062X/6-311++G(d,p), CBS-Q//B3, and G4 calculated gas phase constant pressure heat capacities ($C_{p,gas}$) at 1 atmosphere for the hydroxyl radical between 298.15 and 1500 K. Values in brackets represent percent deviations from experimental data.

T (K)	expt. [12] $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	PM6 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	M062X/6-311++G(d,p) $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	CBS-Q//B3 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	G4 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)
298.15	7.17	6.95 [-2.9%]	6.95 [-3.0%]	6.95 [-3.0%]	6.95 [-3.0%]
300	7.16	6.95 [-2.9%]	6.95 [-2.9%]	6.95 [-2.9%]	6.95 [-2.9%]
500	7.05	7.01 [-0.6%]	6.96 [-1.3%]	6.96 [-1.3%]	6.96 [-1.3%]
700	7.09	7.21 [1.7%]	7.01 [-1.2%]	7.01 [-1.1%]	7.01 [-1.1%]
900	7.23	7.49 [3.5%]	7.13 [-1.4%]	7.14 [-1.3%]	7.14 [-1.3%]
1100	7.44	7.75 [4.2%]	7.31 [-1.7%]	7.33 [-1.5%]	7.33 [-1.5%]
1300	7.66	7.97 [4.1%]	7.50 [-2.0%]	7.53 [-1.8%]	7.53 [-1.7%]
1500	7.88	8.15 [3.5%]	7.69 [-2.3%]	7.71 [-2.0%]	7.72 [-2.0%]

Table 5: Experimental and PM6, CBS-Q//B3, and G4 calculated gas phase constant pressure heat capacities ($C_{p,gas}$) at 1 atmosphere for methane between 298.15 and 1500 K. Values in brackets represent percent deviations from experimental data.

T (K)	expt. [13] $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	PM6 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	CBS-Q//B3 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	G4 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)
298.15	8.53	8.80 [3.2%]	8.46 [-0.9%]	8.45 [-0.9%]
300	8.55	8.83 [3.3%]	8.47 [-0.9%]	8.47 [-0.9%]
400	9.71	10.25 [5.5%]	9.55 [-1.6%]	9.55 [-1.6%]
500	11.14	11.82 [6.1%]	10.90 [-2.2%]	10.90 [-2.2%]
600	12.61	13.33 [5.7%]	12.27 [-2.6%]	12.26 [-2.7%]
700	14.01	14.71 [5.0%]	13.57 [-3.1%]	13.56 [-3.2%]
800	15.32	15.96 [4.2%]	14.78 [-3.5%]	14.76 [-3.7%]
900	16.52	17.07 [3.3%]	15.88 [-3.9%]	15.85 [-4.1%]
1000	17.63	18.05 [2.4%]	16.87 [-4.3%]	16.84 [-4.4%]
1100	18.62	18.90 [1.5%]	17.77 [-4.6%]	17.73 [-4.8%]
1200	19.52	19.65 [0.7%]	18.56 [-4.9%]	18.53 [-5.1%]
1300	20.33	20.30 [-0.2%]	19.27 [-5.2%]	19.23 [-5.4%]
1400	21.06	20.86 [-0.9%]	19.89 [-5.6%]	19.86 [-5.7%]
1500	21.72	21.35 [-1.7%]	20.44 [-5.9%]	20.41 [-6.0%]

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Table 6: Experimental and PM6, CBS-Q//B3, and G4 calculated gas phase constant pressure heat capacities ($C_{p,gas}$) at 1 atmosphere for ethane between 298.15 and 1500 K. Values in brackets represent percent deviations from experimental data.

T (K)	expt. [13] $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	PM6 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	CBS-Q//B3 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	G4 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)
298.15	12.55	12.54 [0.0%]	12.08 [-3.7%]	12.09 [-3.6%]
300	12.60	12.60 [0.0%]	12.13 [-3.7%]	12.14 [-3.6%]
400	15.65	16.02 [2.4%]	15.17 [-3.0%]	15.18 [-3.0%]
500	18.63	19.40 [4.2%]	18.25 [-2.0%]	18.26 [-2.0%]
600	21.32	22.42 [5.2%]	21.05 [-1.2%]	21.06 [-1.2%]
700	23.70	25.05 [5.7%]	23.54 [-0.6%]	23.54 [-0.7%]
800	25.80	27.33 [5.9%]	25.74 [-0.2%]	25.73 [-0.3%]
900	27.66	29.29 [5.9%]	27.69 [0.1%]	27.67 [0.0%]
1000	29.29	30.99 [5.8%]	29.40 [0.4%]	29.37 [0.3%]
1100	30.72	32.45 [5.6%]	30.90 [0.6%]	30.87 [0.5%]
1200	31.98	33.71 [5.4%]	32.22 [0.8%]	32.19 [0.7%]
1300	33.08	34.79 [5.2%]	33.37 [0.9%]	33.34 [0.8%]
1400	34.03	35.72 [5.0%]	34.39 [1.0%]	34.36 [0.9%]
1500	34.87	36.53 [4.8%]	35.27 [1.2%]	35.24 [1.1%]

Table 7: Experimental and PM6, CBS-Q//B3, and G4 calculated gas phase constant pressure heat capacities ($C_{p,gas}$) at 1 atmosphere for propane between 298.15 and 1500 K. Values in brackets represent percent deviations from experimental data.

T (K)	expt. [13] $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	PM6 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	CBS-Q//B3 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	G4 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)
298.15	17.59	17.34 [-1.4%]	16.82 [-4.4%]	16.83 [-4.3%]
300	17.67	17.43 [-1.4%]	16.90 [-4.3%]	16.91 [-4.3%]
400	22.47	22.62 [0.7%]	21.60 [-3.9%]	21.61 [-3.8%]
500	26.91	27.61 [2.6%]	26.19 [-2.7%]	26.20 [-2.6%]
600	30.76	31.99 [4.0%]	30.29 [-1.5%]	30.29 [-1.5%]
700	34.10	35.75 [4.9%]	33.86 [-0.7%]	33.85 [-0.7%]
800	36.99	38.98 [5.4%]	36.98 [0.0%]	36.96 [-0.1%]
900	39.52	41.75 [5.6%]	39.71 [0.5%]	39.68 [0.4%]
1000	41.73	44.12 [5.7%]	42.09 [0.9%]	42.06 [0.8%]
1100	43.66	46.15 [5.7%]	44.17 [1.2%]	44.14 [1.1%]
1200	45.35	47.89 [5.6%]	45.99 [1.4%]	45.95 [1.3%]
1300	46.81	49.39 [5.5%]	47.58 [1.6%]	47.54 [1.6%]
1400	48.09	50.67 [5.4%]	48.96 [1.8%]	48.93 [1.7%]
1500	49.21	51.78 [5.2%]	50.18 [2.0%]	50.14 [1.9%]

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Table 8: Experimental and PM6, CBS-Q//B3, and G4 calculated gas phase constant pressure heat capacities ($C_{p,gas}$) at 1 atmosphere for n-butane between 298.15 and 1500 K. Values in brackets represent percent deviations from experimental data.

T (K)	expt. [13] $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	PM6 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	CBS-Q//B3 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	G4 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)
298.15	23.54	22.25 [-5.5%]	21.64 [-8.1%]	21.65 [-8.0%]
300	23.65	22.37 [-5.4%]	21.75 [-8.0%]	21.76 [-8.0%]
400	29.82	29.26 [-1.9%]	28.03 [-6.0%]	28.05 [-6.0%]
500	35.53	35.83 [0.8%]	34.11 [-4.0%]	34.12 [-4.0%]
600	40.46	41.55 [2.7%]	39.49 [-2.4%]	39.49 [-2.4%]
700	44.70	46.44 [3.9%]	44.15 [-1.2%]	44.14 [-1.3%]
800	48.37	50.62 [4.7%]	48.19 [-0.4%]	48.17 [-0.4%]
900	51.56	54.19 [5.1%]	51.70 [0.3%]	51.67 [0.2%]
1000	54.34	57.24 [5.3%]	54.76 [0.8%]	54.73 [0.7%]
1100	56.76	59.84 [5.4%]	57.42 [1.2%]	57.39 [1.1%]
1200	58.86	62.07 [5.5%]	59.74 [1.5%]	59.70 [1.4%]
1300	60.69	63.98 [5.4%]	61.76 [1.8%]	61.72 [1.7%]
1400	62.28	65.62 [5.4%]	63.53 [2.0%]	63.48 [1.9%]
1500	63.67	67.03 [5.3%]	65.06 [2.2%]	65.02 [2.1%]

Table 9: Experimental and G4 calculated gas phase constant pressure heat capacities ($C_{p,gas}$) at 1 atmosphere for isobutane between 298.15 and 1500 K. Values in brackets represent percent deviations from experimental data.

T (K)	expt. [14] $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	G4 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)
298.15	23.10	22.22 [-3.8%]
300	23.22	22.34 [-3.8%]
500	35.67	34.59 [-3.0%]
700	45.00	44.43 [-1.3%]
900	51.85	51.86 [0.0%]
1100	57.00	57.50 [0.9%]
1300	60.88	61.80 [1.5%]
1500	63.82	65.08 [2.0%]

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Table 10: Experimental and PM6, CBS-Q//B3, and G4 calculated gas phase constant pressure heat capacities ($C_{p,gas}$) at 1 atmosphere for n-pentane between 298.15 and 1500 K. Values in brackets represent percent deviations from experimental data.

T (K)	expt. [13] $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	PM6 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	CBS-Q//B3 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	G4 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)
298.15	28.68	27.18 [-5.2%]	26.53 [-7.5%]	26.54 [-7.5%]
300	28.83	27.34 [-5.2%]	26.67 [-7.5%]	26.67 [-7.5%]
400	36.46	35.90 [-1.5%]	34.51 [-5.3%]	34.52 [-5.3%]
500	43.64	44.04 [0.9%]	42.06 [-3.6%]	42.06 [-3.6%]
600	49.90	51.11 [2.4%]	48.71 [-2.4%]	48.70 [-2.4%]
700	55.30	57.14 [3.3%]	54.44 [-1.5%]	54.43 [-1.6%]
800	59.90	62.26 [3.9%]	59.40 [-0.8%]	59.38 [-0.9%]
900	63.80	66.63 [4.4%]	63.70 [-0.2%]	63.67 [-0.2%]
1000	67.30	70.35 [4.5%]	67.43 [0.2%]	67.39 [0.1%]
1100	70.20	73.53 [4.7%]	70.68 [0.7%]	70.63 [0.6%]
1200	72.80	76.24 [4.7%]	73.50 [1.0%]	73.45 [0.9%]
1300	75.00	78.57 [4.8%]	75.95 [1.3%]	75.90 [1.2%]
1400	77.00	80.56 [4.6%]	78.09 [1.4%]	78.04 [1.3%]
1500	79.00	82.28 [4.1%]	79.95 [1.2%]	79.91 [1.1%]

Table 11: Experimental and PM6 and CBS-Q//B3 calculated gas phase constant pressure heat capacities ($C_{p,gas}$) at 1 atmosphere for n-hexane between 298.15 and 1500 K. Values in brackets represent percent deviations from experimental data.

T (K)	expt. [13] $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	PM6 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	CBS-Q//B3 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)
298.15	34.08	32.12 [-5.8%]	31.39 [-7.9%]
300	34.24	32.30 [-5.7%]	31.56 [-7.8%]
400	43.39	42.54 [-1.9%]	40.97 [-5.6%]
500	51.93	52.26 [0.6%]	49.99 [-3.7%]
600	59.30	60.67 [2.3%]	57.92 [-2.3%]
700	65.50	67.83 [3.6%]	64.74 [-1.2%]
800	70.80	73.90 [4.4%]	70.61 [-0.3%]
900	75.30	79.07 [5.0%]	75.70 [0.5%]
1000	79.20	83.47 [5.4%]	80.10 [1.1%]
1100	82.50	87.22 [5.7%]	83.93 [1.7%]
1200	85.40	90.42 [5.9%]	87.25 [2.2%]
1300	88.00	93.15 [5.9%]	90.14 [2.4%]
1400	90.00	95.50 [6.1%]	92.65 [2.9%]
1500	93.00	97.52 [4.9%]	94.84 [2.0%]

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Table 12: Experimental and PM6 and CBS-Q//B3 calculated gas phase constant pressure heat capacities ($C_{p,gas}$) at 1 atmosphere for n-heptane between 298.15 and 1500 K. Values in brackets represent percent deviations from experimental data.

T (K)	expt. [13] $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	PM6 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	CBS-Q//B3 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)
298.15	39.48	37.05 [-6.2%]	36.25 [-8.2%]
300	39.67	37.26 [-6.1%]	36.45 [-8.1%]
400	50.35	49.19 [-2.3%]	47.43 [-5.8%]
500	60.25	60.47 [0.4%]	57.93 [-3.9%]
600	68.70	70.23 [2.2%]	67.13 [-2.3%]
700	75.80	78.52 [3.6%]	75.03 [-1.0%]
800	81.80	85.55 [4.6%]	81.83 [0.0%]
900	86.90	91.51 [5.3%]	87.69 [0.9%]
1000	91.20	96.59 [5.9%]	92.78 [1.7%]
1100	94.90	100.91 [6.3%]	97.18 [2.4%]
1200	98.10	104.59 [6.6%]	101.00 [3.0%]
1300	101.00	107.74 [6.7%]	104.32 [3.3%]
1400	104.00	110.44 [6.2%]	107.21 [3.1%]
1500	106.00	112.77 [6.4%]	109.73 [3.5%]

Table 13: Experimental and PM6 and CBS-Q//B3 calculated gas phase constant pressure heat capacities ($C_{p,gas}$) at 1 atmosphere for n-octane between 298.15 and 1500 K. Values in brackets represent percent deviations from experimental data.

T (K)	expt. [13] $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	PM6 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	CBS-Q//B3 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)
298.15	44.89	41.99 [-6.4%]	41.12 [-8.4%]
300	45.10	42.23 [-6.4%]	41.34 [-8.3%]
400	57.30	55.84 [-2.6%]	53.89 [-5.9%]
500	68.55	68.69 [0.2%]	65.87 [-3.9%]
600	78.10	79.80 [2.2%]	76.35 [-2.2%]
700	86.10	89.21 [3.6%]	85.33 [-0.9%]
800	92.80	97.19 [4.7%]	93.05 [0.3%]
900	98.40	103.96 [5.6%]	99.70 [1.3%]
1000	103.10	109.71 [6.4%]	105.46 [2.3%]
1100	107.20	114.60 [6.9%]	110.44 [3.0%]
1200	110.70	118.77 [7.3%]	114.77 [3.7%]
1300	114.00	122.33 [7.3%]	118.52 [4.0%]
1400	117.00	125.39 [7.2%]	121.78 [4.1%]
1500	119.00	128.02 [7.6%]	124.63 [4.7%]

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Table 14: Experimental and PM6 and CBS-Q//B3 calculated gas phase constant pressure heat capacities ($C_{p,gas}$) at 1 atmosphere for n-nonane between 298.15 and 1500 K. Values in brackets represent percent deviations from experimental data.

T (K)	expt. [13] $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	PM6 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	CBS-Q//B3 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)
298.15	50.29	46.93 [-6.7%]	45.97 [-8.6%]
300	50.53	47.20 [-6.6%]	46.22 [-8.5%]
400	64.25	62.48 [-2.7%]	60.34 [-6.1%]
500	76.85	76.91 [0.1%]	73.81 [-4.0%]
600	87.50	89.36 [2.1%]	85.56 [-2.2%]
700	96.40	99.91 [3.6%]	95.62 [-0.8%]
800	103.70	108.83 [4.9%]	104.26 [0.5%]
900	109.90	116.40 [5.9%]	111.70 [1.6%]
1000	115.10	122.82 [6.7%]	118.13 [2.6%]
1100	119.50	128.29 [7.4%]	123.69 [3.5%]
1200	123.40	132.94 [7.7%]	128.52 [4.1%]
1300	127.00	136.92 [7.8%]	132.70 [4.5%]
1400	130.00	140.33 [7.9%]	136.34 [4.9%]
1500	133.00	143.26 [7.7%]	139.51 [4.9%]

Table 15: Experimental and PM6 calculated gas phase constant pressure heat capacities ($C_{p,gas}$) at 1 atmosphere for n-decane between 298.15 and 1500 K. Values in brackets represent percent deviations from experimental data.

T (K)	expt. $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)	PM6 $C_{p,gas}$ (cal mol ⁻¹ K ⁻¹)
298.15	55.71	51.86 [-6.9%]
300	55.97	52.17 [-6.8%]
400	71.22	69.13 [-2.9%]
500	85.19	85.13 [-0.1%]
600	97.00	98.92 [2.0%]
700	106.70	110.60 [3.7%]
800	114.70	120.47 [5.0%]
900	121.50	128.84 [6.0%]
1000	127.10	135.94 [7.0%]
1100	131.90	141.98 [7.6%]
1200	136.10	147.12 [8.1%]
1300	140.00	151.51 [8.2%]
1400	143.00	155.27 [8.6%]
1500	146.00	158.51 [8.6%]

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