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Low-temperature heat capacities and standard molar enthalpy of formation of 4-(2-aminoethyl)-phenol ($C_8H_{11}NO$)*

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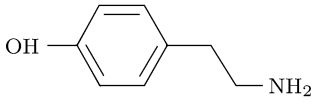
This paper reports that low-temperature heat capacities of 4-(2-aminoethyl)-phenol ($C_8H_{11}NO$) are measured by a precision automated adiabatic calorimeter over the temperature range from 78 to 400 K. A polynomial equation of heat capacities as a function of the temperature was fitted by the least square method. Based on the fitted polynomial, the smoothed heat capacities and thermodynamic functions of the compound relative to the standard reference temperature 298.15 K were calculated and tabulated at the interval of 5 K. The energy equivalent, $\varepsilon_{\rm calor}$, of the oxygen-bomb combustion calorimeter has been determined from 0.68 g of NIST 39i benzoic acid to be $\varepsilon_{\rm calor}$=(14674.69±17.49)J·K^{-1}. The constant-volume energy of combustion of the compound at T=298.15 K was measured by a precision oxygen-bomb combustion calorimeter to be $\Delta_{\rm c}U$=–(32374.25±12.93)J·g^{-1}. The standard molar enthalpy of combustion for the compound was calculated to be $\Delta_{\rm c}H_{\rm m}^{\ominus} = -(4445.47 \pm 1.77)\,{\rm kJ\cdot mol^{-1}}$ according to the definition of enthalpy of combustion and other thermodynamic principles. Finally, the standard molar enthalpy of formation of the compound was derived to be $\Delta_{\rm f}H_{\rm m}^{\ominus}({\rm C_8H_{11}NO, s}) = -(274.68 \pm 2.06)\,{\rm kJ\cdot mol^{-1}}$, in accordance with Hess law.

Keywords: 4-(2-aminoethyl)-phenol, adiabatic calorimetry, low-temperature heat capacity, standard molar enthalpy of formation

PACC: 0570, 8260

1. Introduction

4-(2-aminoethyl)-phenol (CAS registry number, 51-67-2; Beilstein number, 1099914) is also called as the tyramine, tyrosamine, tocosine and uteramine. It is an important alkaloid, able to relax or spread the blood vessel of the human body, and an intermediate and rude material in preparing the drugs curing the cardiovascular diseases. In addition, the compound plays an important role in radiation hardening, antifungal and activating nerve centre of the respiratory system. Its boiling point ($T_{\rm boil}$) is 451.2 K at the pressure of 0.01 Bar. The solubility of the compound in water is 1.05 g/100 mL water at T=288.15 K.[1] Its molecular structure is,



The heat capacity and standard molar enthalpy of formation of a substance are the most fundamental thermodynamic properties and closely related to other physical, biological, physiological and chemical properties.[2–8] These results play an important role in calculating enthalpy change, equilibrium constant, and theoretical yield of the chemical reaction in which the substance was involved. However, up until now, no report about thermodynamic properties of 4-(2-aminoethyl)-phenol was found in literatures. In the present work, heat capacities, thermodynamic properties and the standard molar enthalpy of formation of the compound have been investigated by adiabatic calorimetry and combustion calorimetry.

2. Experimental

2.1. Sample

The sample used in these calorimetric measurements was purchased from Alfa Aesar (Tianjin, China)

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Co., Ltd. The labelled purity is more than 99.0%. The melting point was measured to be 163–165°C, as measured by micro melting point device. The actual purity of the sample was determined to be more than 99.5% by high performance liquid chromatography (HPLC). At last, Fourier transform infrared spectroscopy (FTIR) and H^1 nuclear magnetic resonance (NMR) were applied to verify the structure of the compound.

2.2. Adiabatic calorimetry

A high-precision automatic adiabatic calorimeter with a small sample size was applied to measure the heat capacities in the temperature range from T=78 K to T=400 K. The principle and design of the adiabatic calorimeter were described in detail elsewhere.[9,10] Briefly, the calorimeter mainly comprised a sample cell, a platinum resistance thermometer, an electric heater, the inner and the outer adiabatic shields, and a vacuum can. Two sets of six-junction chromel-constantan thermopiles installed between the calorimetric cell and the inner shield and between the inner and outer shields, respectively. The miniature platinum resistance thermometer (IPRT No.2, produced by the Shanghai Institute of Industrial Automatic Meters, 16 mm in length, 1.6 mm in diameter and a nominal resistance of 100 Ω) was applied to measure the temperature of the sample. The thermometer was calibrated on the basis of ITS-90 by the Station of Low-temperature Metrology and Measurements, Chinese Academy of Sciences. The thermometer was inserted into the copper sheath which was silver-soldered closely at the bottom of the sample cell. The temperature differences between the sample cell and the inner shield and between the inner and outer shields were monitored by two sets of thermopiles, and controlled by two sets of DWT-702 precision temperature controllers (manufactured by Shanghai No.6 Automated Instrumentation Works). The vacuum can was evacuated to 100 Pa during the heat capacity measurements so as to eliminate heat transfer by convection. The electrical energy introduced into the sample cell and the equilibrium temperature of the cell after the energy input were automatically picked up by use of the Data Acquisition / Switch Unit (Model 34970A, Agilent, USA), and processed on line by a computer.

To verify the accuracy of the calorimeter, the heat-capacity measurements of the reference standard material, α-Al_2O_3, were made in the temperature range from T=78 K to T=400 K. The sample mass used was 1.6382 g, which was equivalent to 0.0161 mol based on its molar mass, M (Al_2O_3)=101.9613 g·mol^{-1}. The results indicated that deviations of the experimental data from those of the former National Bureau of Standards[11] in the same temperature range were within ±0.3 %.

Heat-capacity measurements were continuously and automatically carried out by means of the standard method of intermittently heating the sample and alternately measuring the temperature. The heating rate and the temperature increments were generally controlled at (0.1 to 0.4) K·min^{-1} and (1 to 3) K. The heating duration was 10 min, and the temperature drift rates of the sample cell measured in an equilibrium period were always kept within (10^{-3} to 10^{-4}) K·min^{-1} during the acquisition of all heat-capacity data. The sample mass used for the calorimetric measurements was 2.2729 g, which was equivalent to 0.01657 mol in terms of molar mass of the sample, 4-(2-aminoethyl)-phenol, $C_8H_{11}NO$(s), M=137.181 g· mol^{-1}.

2.3. Isoperibol oxygen-bomb combustion calorimetry

The constant-volume energy of combustion of the sample was measured by means of a homemade precision oxygen-bomb combustion calorimeter. It was an isoperibolic macrocalorimeter with a static oxygen bomb and set up in our thermochemistry laboratory. The structure and principle of the calorimeter have been described in detail previously elsewhere.[12,13] It consisted of a static oxygen bomb, inner calorimetric vessel, outer thermostatic bath, platinum resistance thermometer, precision temperature controller, ignition system and temperature measurement system. The system of controlling the temperature was composed of a thermostatic bath, an electric stirrer, an electric heater, a precision temperature controller and a Cu 50 resistance thermometer. The precision of controlling the temperature for the thermostatic system can reach ±0.001 K.

The temperature measurement system consisted of a precision platinum resistance thermometer

(PTΦ5×40, 40 mm in length, 5 mm in diameter; R_0=196.9865 Ω, made by the Instrument Manufacture Co. of Yunnan, China) and a Data Acquisition / Switch Unit (Model 34970A, Agilent, USA). The thermometer was calibrated on the basis of ITS-90 by the National Institute of Metrology.

The correction of the temperature rise (ς) was obtained from a formula described in the Refs.[12–14].

The sample was pressed into pellets of (0.6 to 1.0) g for each combustion and burned under an oxygen pressure of 3.01 MPa in the presence of 0.001 dm^3 of distilled water in the bomb to ensure equilibrium in the final state after the combustion. The purity of the oxygen used in the experiment was of research grade, mole fraction 0.99998. The mass of the sample has been calibrated from the air buoyancy on the basis of the determination of the density for a pellet of the sample. At T=(298.15 ± 0.001) K, the differential quotient of the constant-volume energy of combustion with the oxygen pressure, $(\partial U/\partial P)_T$, for the solid was assumed to be –0.21 $J\cdot g^{-1}\cdot MPa^{-1}$, a typical value for organic solids. Corrected value of the energy of combustion for the pressure in the oxygen bomb from 3 MPa to 100 kPa was estimated to be 0.60 $J\cdot g^{-1}$ and can be omitted. The standard energy of combustion of the nickel fuse for ignition has been determined previously to be $\Delta_c U^\circ/J\cdot cm^{-1}$=2.929. The real energy of combustion of the nickel fuse (Q_{Ni}) was calculated from the formula, Q_{Ni}/J=2.929·ΔL, in which ΔL /cm was the length of the combusted nickel wire. The correction for the energy of formation of aqueous nitric acid, produced by oxidation of a trace of nitrogen contained in the oxygen bomb, was determined by the neutral titration with a 0.1000 $mol\cdot dm^{-3}$ of sodium hydroxide solution by using the methyl orange as the indicator. The heat of formation of the aqueous nitric acid in the oxygen bomb can be derived from the equation, $Q_{HNO3}/J = 59.8\cdot N\cdot V$, in which $N/(mol\cdot dm^{-3})$ is the concentration of the sodium hydroxide solution and V/cm^3 is the volume of the consumed sodium hydroxide solution, based on the molar energy of formation of HNO_3(aq) from N_2(g), O_2(g) and H_2O(l), $\Delta_f H^0_m$=59.8 $kJ\cdot mol^{-1}$,[12,14] for 0.1 $mol\cdot dm^{-3}$ of HNO_3(aq).

After each combustion test, the combustion products were analysed mainly for carbon dioxide by the Rossini method.[12,14] No soot was observed in the sample crucible after each of combustion experiments for 4-(2-aminoethyl)-phenol ($C_8H_{11}NO$). Qualitative tests for CO with indicator tubes were negative within the limits of their sensitivity (mole fraction x (CO)< 1×10^{-6}).

A new oxygen bomb was used for determination of the combustion heat of the sample. The energy equivalent, ε_{calor}, of the calorimeter has been determined from 0.68 g of NIST 39i benzoic acid with a certified massic energy of combustion under experimental conditions of $\Delta_c U = -(26434\pm3)\ J\cdot g^{-1}$ based on the following formula, in which the subscript c denotes the combustion:

$$\varepsilon_{calor} = \left(\frac{\Delta_c U \cdot W + Q_{Ni} + Q_{HNO_3}}{\Delta T}\right), \qquad (1)$$

which is ε_{calor}=(14674.69± 17.49) $J\cdot K^{-1}$, as indicated in Table 1. The uncertainty of the results was the standard deviation of the mean value from the respective measurements.

Table 1. The energy equivalent (ε_{calor}) of the calorimeter determined from combustion experiments using NIST 39i benzoic acid.

No.	W/g	Q_{Ni}/J	Q_{HNO_3}/J	ΔT/K	$\varepsilon_{calor}/(J\cdot K^{-1})$
1	0.68831	42.468	22.848	1.2424	14697.44
2	0.67416	41.589	21.290	1.2258	14589.35
3	0.68121	43.639	20.511	1.2277	14719.60
4	0.68036	41.003	16.617	1.2284	14687.61
5	0.67285	41.296	22.329	1.2135	14709.31
6	0.69058	43.867	22.989	1.2486	14673.75
7	0.67988	41.786	21.467	1.2257	14714.20
8	0.66896	41.106	21.908	1.2148	14608.42
$\varepsilon_{calor}/(J\cdot K^{-1})$=(14674.69± 17.49)					

3. Results and discussion

3.1. Low-temperature heat capacity

All experimental heat-capacity values tabulated in Table 2 and plotted in Fig.1, show that the structure of the compound was stable over the temperature range between T=78 K and T=400 K, that is, no phase change, association nor thermal decomposition occurred. The 98 experimental points in the temperature region between T=78 K and T=400 K were fitted by means of the least squares method and a polynomial equation of the experimental molar heat capacities ($C_{p,m}$) vs reduced temperature (X), $X = f(T) = \left[T/\mathrm{K} - \frac{1}{2}(T_1 + T_2)\right] \Big/ \left[\frac{1}{2}(T_1 - T_2)\right]$ (where T_1=400 K and T_2=78 K), has been obtained,

The experimental molar heat capacities ($\mathrm{J\cdot K^{-1}\cdot mol^{-1}}$) in the temperature range of 78–400 K were fitted to:

$$C_{p,m} = 166.635 + 123.521X + 15.504X^2 - 6.193X^3 - 2.792X^4,$$

in which, X=(T/K–239)/161, the subscript p and m denote the constant pressure and molar heat capacity, respectively. The standard deviations of experimental molar heat capacities from the smoothed heat capacities calculated by the polynomial equation were within ±0.3% except for several points around the lower and upper temperature limits. The coefficient of determination for the fitting R^2 equals 0.99995. The uncertainties of the coefficients of the equation have been determined to be 0.09%, 0.6%, 0.75%, 0.96%, and 1.5%, respectively.

Table 2. Experimental molar heat capacities of 4-(2-aminoethyl)-phenol ($C_8H_{11}NO$) (M=137.181 $\mathrm{g\cdot mol^{-1}}$).

T/K	$C_{p,m}$ /($\mathrm{J\cdot K^{-1}\cdot mol^{-1}}$)	T/K	$C_{p,m}$ /($\mathrm{J\cdot K^{-1}\cdot mol^{-1}}$)	T/K	$C_{p,m}$ /($\mathrm{J\cdot K^{-1}\cdot mol^{-1}}$)
78.676	62.29	175.660	120.49	298.347	213.72
80.962	63.65	178.778	122.82	301.866	216.99
83.239	64.88	181.937	124.77	305.384	220.16
85.518	65.92	185.056	127.21	309.098	223.17
87.819	67.01	188.894	129.70	312.421	225.98
90.089	68.19	192.332	132.03	315.940	229.15
92.106	69.44	195.451	134.40	319.849	232.36
95.080	71.11	198.570	136.54	323.367	235.23
97.799	72.72	202.448	139.10	327.326	238.34
100.358	74.11	206.326	142.32	330.600	241.11
102.949	75.56	209.725	144.76	334.753	244.37
105.572	77.23	213.163	147.55	338.663	247.24
108.770	79.11	217.321	150.69	342.599	250.39
111.777	80.86	220.893	153.10	345.544	252.88
114.656	82.52	224.020	155.46	348.461	255.11
117.630	84.27	228.214	158.60	351.291	257.47
121.053	86.32	231.910	161.55	354.207	259.83
124.603	88.50	235.789	164.28	357.008	261.96
127.898	90.61	239.658	167.29	359.693	264.02
131.032	92.57	243.527	170.15	362.263	265.85
134.438	94.49	247.086	172.67	364.833	267.95
137.717	96.32	250.604	175.24	367.519	270.18
140.995	98.31	254.318	178.20	370.349	272.61
144.114	100.03	258.276	181.16	373.872	275.55
147.072	102.02	261.550	183.98	377.048	278.04
150.071	103.82	265.264	186.99	380.484	280.96
153.030	105.77	269.614	190.31	384.007	283.78
155.549	107.53	274.402	194.08	387.068	286.20
158.827	109.32	278.116	197.24	390.129	288.99
161.826	111.23	281.830	200.56	393.305	291.81
164.825	113.30	286.179	203.93	396.222	294.59
167.943	115.40	290.284	207.34	399.283	297.21
171.502	117.70	294.243	210.31		

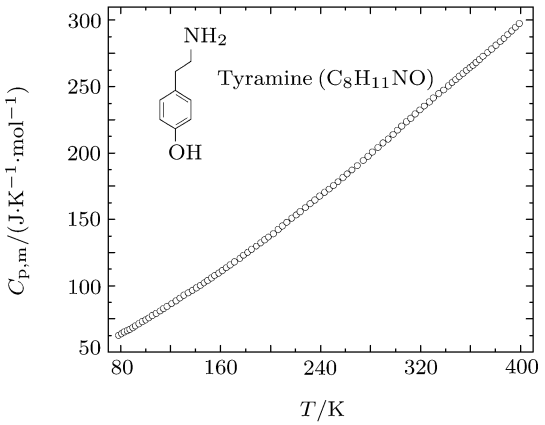


Fig.1. The curve of the experimental molar heat capacities of 4-(2-aminoethyl)-phenol ($C_8H_{11}NO$).

3.2. Thermodynamic functions of the compound

The smoothed molar heat capacities and thermodynamic functions of 4-(2-aminoethyl)-phenol ($C_8H_{11}NO$) were calculated based on a fitted polynomial of the heat capacities as a function of the reduced temperature (X) according to the following thermodynamic equations:

$$(H_T - H_{298.15}) = \int_{298.15}^{T} C_p dT, \quad (2)$$

$$(S_T - S_{298.15}) = \int_{298.15}^{T} C_p \cdot T^{-1} dT, \quad (3)$$

$$(G_T - G_{298.15}) = \int_{298.15}^{T} C_p dT - T\int_{298.15}^{T} C_p \cdot T^{-1} dT. \quad (4)$$

The polynomial fitted values of the molar heat capacities and fundamental thermodynamic functions of the sample relative to the standard reference temperature 298.15 K were tabulated in Table 3 with the interval of 5 K.

Table 3. Thermodynamic functions of 4-(2-aminoethyl)-phenol ($C_8H_{11}NO$)(s) (M=137.181 g·mol^{-1}).

T/K	$C_{p,m}$ /(J·K^{-1}·mol^{-1})	$(H_T - H_{298.15K})$/ (kJ·mol^{-1})	$(S_T - S_{298.15K})$ /(J·K^{-1}·mol^{-1})	$(G_T - G_{298.15K})$ /(kJ·mol^{-1})
80	63.08	–28.99	–154.0	–16.66
85	65.75	–28.66	–150.1	–15.90
90	68.46	–28.33	–146.3	–15.16
95	71.20	–27.98	–142.5	–14.44
100	73.98	–27.62	–138.8	–13.74
105	76.80	–27.24	–135.1	–13.05
110	79.65	–26.85	–131.5	–12.39
115	82.55	–26.44	–127.8	–11.74
120	85.47	–26.02	–124.3	–11.11
125	88.44	–25.59	–120.7	–10.50
130	91.45	–25.14	–117.2	–9.907
135	94.50	–24.67	–113.6	–9.331
140	97.58	–24.19	–110.2	–8.772
145	100.71	–23.70	–106.7	–8.230
150	103.88	–23.19	–103.2	–7.705
155	107.08	–22.66	–99.75	–7.197
160	110.33	–22.11	–96.31	–6.706
165	113.61	–21.56	–92.87	–6.232
170	116.94	–20.98	–89.44	–5.775
175	120.30	–20.39	–86.01	–5.335
180	123.71	–19.78	–82.58	–4.912
185	127.15	–19.15	–79.15	–4.506
190	130.63	–18.50	–75.72	–4.117
195	134.15	–17.84	–72.29	–3.746
200	137.70	–17.16	–68.86	–3.391
205	141.29	–16.47	–65.42	–3.054

Table 3. (*Continued*).

T/K	$C_{p,m}$ /(J·K^{-1}·mol^{-1})	$(H_T - H_{298.15K})$/ (kJ·mol^{-1})	$(S_T - S_{298.15K})$ /(J·K^{-1}·mol^{-1})	$(G_T - G_{298.15K})$ /(kJ·mol^{-1})
210	144.92	–15.75	–61.98	–2.735
215	148.59	–15.02	–58.53	–2.433
220	152.28	–14.26	–55.07	–2.148
225	156.02	–13.49	–51.61	–1.881
230	159.78	–12.70	–48.14	–1.632
235	163.58	–11.90	–44.66	–1.400
240	167.40	–11.07	–41.18	–1.186
245	171.26	–10.22	–37.68	–0.9892
250	175.14	–9.355	–34.18	–0.8105
255	179.06	–8.470	–30.67	–0.6496
260	183.00	–7.564	–27.15	–0.5065
265	186.96	–6.640	–23.62	–0.3811
270	190.95	–5.695	–20.08	–0.2736
275	194.95	–4.730	–16.53	–0.1839
280	198.98	–3.745	–12.98	–0.1119
285	203.03	–2.740	–9.412	–0.0577
290	207.09	–1.715	–5.840	–0.0213
295	211.17	–0.6692	–2.260	–0.0027
298.15	213.75	0	0	0
300	215.27	0.3968	1.329	–0.0017
305	219.37	1.483	4.924	–0.0185
310	223.49	2.591	8.528	–0.0530
315	227.61	3.718	12.14	–0.1052
320	231.74	4.867	15.76	–0.1751
325	235.87	6.036	19.38	–0.2627
330	240.00	7.225	23.01	–0.3680
335	244.13	8.436	26.65	–0.4911
340	248.26	9.667	30.29	–0.6320
345	252.39	10.92	33.94	–0.7907
350	256.50	12.19	37.59	–0.9673
355	260.61	13.48	41.25	–1.162
360	264.70	14.80	44.92	–1.375
365	268.78	16.13	48.59	–1.606
370	272.84	17.48	52.27	–1.856
375	276.88	18.86	55.95	–2.124
380	280.90	20.25	59.64	–2.412
385	284.89	21.67	63.34	–2.719
390	288.85	23.10	67.04	–3.045
395	292.78	24.56	70.75	–3.392
400	296.67	26.03	74.47	–3.759

3.3. Constant-volume energy of combustion and standard molar enthalpy of combustion of the compound

The method for determining the constant-volume energy of combustion of the sample was the same as that used in the calibration of the combustion calorimeter with benzoic acid. The constant-volume energy of combustion of the sample can be calculated according to the formula in Refs.[12] and [14].

$$\Delta_c U = \left(\frac{\varepsilon_{\text{calor}} \cdot \Delta T - Q_{\text{Ni}} - Q_{\text{HNO}_3}}{W} \right). \quad (5)$$

The measured result of the constant-volume energy ($\Delta_c U$) of combustion of the sample was indicated in Table 4.

Table 4. The experimental results of the constant-volume energy of combustion for 4-(2-aminoethyl)-phenol ($C_8H_{11}NO$) at 298.15 K and 0.1 MPa.

No	Mass of sample W/g	Corrected heat of ignition wire Q_c/J	Corrected heat of nitric acid Q_N/J	Corrected temperature rise $\Delta_c T$/K	Combustion energy of sample $-\Delta_c U/(J\cdot g^{-1})$
1	0.56571	43.639	44.138	1.2567	32444.02
2	0.54351	42.760	43.099	1.2094	32495.65
3	0.53577	41.003	41.023	1.1876	32375.15
4	0.54289	43.932	41.023	1.1999	32277.64
5	0.54378	45.689	42.061	1.1978	32163.00
6	0.55373	43.467	43.439	1.2249	32304.77
7	0.54896	43.768	42.687	1.2118	32236.11
8	0.53982	42.496	41.698	1.2006	32481.64
Mean: $\Delta_c U = -(32374.25\pm12.93)\ J\cdot g^{-1}$					

The standard molar enthalpy of combustion of the sample ($\Delta_c H_m^{\ominus}$) referred to the enthalpy change of the following reaction at 298.15 K and 100 kPa,

$$\begin{aligned} &C_8H_{11}NO(s) + \frac{41}{4}O_2(g) \\ =&8CO_2(g) + \frac{11}{2}H_2O(l) + \frac{1}{2}N_2(g). \end{aligned} \tag{6}$$

The standard molar enthalpy of combustion of the sample can be derived from the constant-volume energy of combustion by Eqs.(7) and (8):

$$\Delta_c H_m^{\ominus} = \Delta_c U_m^{\ominus} + \Delta n \cdot RT, \tag{7}$$

$$\Delta n = \Sigma n_i(\text{products, g}) - \Sigma n_i(\text{reactants, g}), \tag{8}$$

where Σn_i was the total amount (in moles) of the gases presented as products or as reactants. The calculated standard molar enthalpy of combustion of the sample was calculated, the unit of $\Delta_c U$ was conversed from $J\cdot g^{-1}$ to $kJ\cdot mol^{-1}$, $\Delta_c U_m^{\ominus} = -(4441.13\pm 1.77)\ kJ\cdot mol^{-1}$, then according to $\Delta n = -1.75$,

$$\begin{aligned} \Delta_c H_m^{\ominus} =&\Delta_c U_m^{\ominus} + \Delta n \cdot RT \\ =&-(4445.47 \pm 1.77)\ kJ\cdot mol^{-1}. \end{aligned}$$

3.4. Standard molar enthalpy of formation of the compound

A reaction scheme used to determine the standard molar enthalpy of formation of 4-(2-aminoethyl)-phenol ($C_8H_{11}NO$) was shown in Table 5, and $\Delta_f H_m^o(C_8H_{11}NO, s)$ (in which the subscript f denotes the formation and H denotes the enthalpy) was calculated by a designed Hess's thermochemical cycle according to the reaction Eq.(6) as follows:

$$\begin{aligned} \Delta H_4 =&\Delta_f H_m^{\ominus}(C_8H_{11}NO, s) \\ =&8\Delta_f H_m^{\ominus}(CO_2, g) + \frac{11}{2}\Delta_f H_m^{\ominus}(H_2O, l) \\ &-\Delta_c H_m^{\ominus}\ (C_8H_{11}NO, s) \\ =&8\Delta H_2 + \frac{11}{2}\Delta H_3 - \Delta H_1. \end{aligned} \tag{9}$$

In Eq.(9), the standard molar enthalpies of formation of CO_2 (g) and H_2O (l), recommended by CODATA,[15,16] $\Delta_f H_m^{\ominus}(CO_2, g) = -(393.51 \pm 0.13)\ kJ\cdot mol^{-1}$ and $\Delta_f H_m^{\ominus}(H_2O, l) = -(285.83 \pm 0.04)\ kJ\cdot mol^{-1}$, were employed in the calculation of $\Delta_f H_m^{\ominus}[C_8H_{11}NO, s]$. The standard molar enthalpy of formation of the compound can be derived to be $\Delta_f H_m^{\ominus}(C_8H_{11}NO, s) = -(274.68 \pm 2.06)\ kJ\cdot mol^{-1}$.

Table 5. Reaction scheme used to determine the standard molar enthalpy of formation of 4-(2-aminoethyl)-phenol ($C_8H_{11}NO$).

No.	reactions	$\Delta_f H_m^{\ominus}$ or $(\Delta_c H_m^{\ominus} \pm \sigma_a)/(kJ\cdot mol^{-1})$
1	$C_8H_{11}NO(s) + \frac{41}{4}O_2(g) = 8CO_2(g) + \frac{11}{2}H_2O(l) + \frac{1}{2}N_2(g)$	–(4445.47 ± 1.77), ΔH_1
2	O_2 (g) + C (s) = CO_2 (g)	–(393.51 ± 0.13), ΔH_2
3	H_2 (g) + 1/2O_2 (g) = H_2O (l)	–(285.83 ± 0.04), ΔH_3
4	$8C(s) + \frac{11}{2}H_2(g) + \frac{1}{2}O_2(g) + \frac{1}{2}N_2(g) = C_8H_{11}NO(s)$	–(274.68 ± 2.06), ΔH_4

Here $\sigma_a = \frac{\sigma}{\sqrt{n}} = \frac{\sqrt{\sum_{i=1}^{n}(x_i - \overline{x})^2/(n-1)}}{\sqrt{n}} = \sqrt{\sum_{i=1}^{n}(x_i - \overline{x})^2/n(n-1)}$, in which n is the experimental number; x_i, a single value obtained from a series of measurements; $\overline{x}$, the mean value of the results.

4. Conclusion

This paper reported low-temperature heat capacities and constant-volume energy of combustion of 4-(2-aminoethyl)-phenol measured by adiabatic calorimetry and isoperibol oxygen-bomb combustion calorimetry. Additionally, thermodynamic parameters of the thermodynamic functions and standard molar enthalpy of formation of the compound were derived from these experimental results.

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