

Supporting Materials

# The Vaporization Enthalpy and Vapor Pressure of (±)-N-Ethylamphetamine at $T/K = 298.15$ by Correlation Gas Chromatography

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**Table S1. A:** Retention times of N-ethylamphetamine and compounds used as standards.

Run 1	T/K	392.9	397.9	403	408.1	413.1	418.1	423.2
Methanol		0.517	0.525	0.529	0.524	0.062	0.538	0.542
N,N-Di-n-butylamine		1.261	1.172	1.095	1.020	0.500	0.928	0.887
N,N-Di-n-pentylamine		2.879	2.518	2.223	1.967	1.300	1.611	1.470
N-Ethylamphetamine		4.434	3.814	3.317	2.891	2.083	2.285	2.048
N,N-Di-n-hexylamine		7.893	6.562	5.524	4.656	3.507	3.453	2.992
4-Benzylpiperidine		17.772	14.578	12.128	10.094	7.999	7.239	6.157
N,N-Di-n-heptylamine		23.179	18.485	14.970	12.139	9.482	8.321	6.930

**Table S1. B:** Correlation between  $\Delta_l^g H_m(298.15 \text{ K})$  and  $\Delta H_{\text{trn}}(408\text{K})$  of the standards<sup>1</sup>

Run 1	-slope T/K	intercept	$\Delta H_{\text{trn}}(408\text{K})$ kJ·mol <sup>-1</sup>	$\Delta_l^g H_m(298.15 \text{ K})/\text{kJ·mol}^{-1}$ (lit) <sup>2</sup>	(calc)
N,N-Di-n-butylamine	4197.2±20	10.984±0.05	34.89±0.16	50.1±0.6	50.4±3.4
N,N-Di-n-pentylamine	5121.3±23	12.181±0.06	42.58±0.19	61.3±2.1	61.0±3.7
N-Ethylamphetamine	5238.1±24	11.973±0.06	43.55±0.20		62.4±3.8
N,N-Di-n-hexylamine	6037.1±24	13.374±0.06	50.19±0.20	70.7±3.4	71.5±4.0
4-Benzylpiperidine	6149.2±27	12.810±0.07	51.12±0.22	74.2±1.0	72.8±4.1
N,N-Di-n-heptylamine	6937.5±36	14.546±0.09	57.68±0.30	81.3±4.9	81.8±4.3

$$\Delta_l^g H_m(298.15 \text{ K})/\text{kJ·mol}^{-1} = (1.38 \pm 0.06) \Delta H_{\text{trn}}(408 \text{ K}) + (2.3 \pm 2.8) \quad r^2 = 0.9947 \quad (\text{S1})$$

<sup>1</sup> All uncertainties represent one standard deviation.

<sup>2</sup> Vaporization enthalpies are average literature values; individual values and references are reported in Table 2.

**Table S2. A:** Retention times of N-ethylamphetamine and compounds used as standards.

Run 2	392.9	398	403.1	408.2 t/min	413.2	418.2	423.2
Methanol	0.541	0.536	0.551	0.545	0.549	0.557	0.559
N,N-Di-n-butylamine	1.315	1.211	1.142	1.049	1.006	0.960	0.919
N,N-Di-n-pentylamine	2.998	2.613	2.318	2.035	1.842	1.670	1.527
N-Ethylamphetamine	4.614	3.966	3.459	2.996	2.663	2.371	2.130
N,N-Di-n-hexylamine	18.524	15.237	12.648	10.488	8.871	7.495	6.405
4-Benzylpiperidine	24.132	19.318	15.625	12.647	10.437	8.624	7.212
N,N-Di-n-heptylamine	24.132	19.318	15.625	12.647	10.437	8.624	7.212

**Table S2. B:** Correlation between  $\Delta_l^g H_m(298.15\text{ K})$  and  $\Delta H_{\text{tm}}(408\text{ K})$  of the standards <sup>1</sup>

Run 2	-slope T/K	intercept	$\Delta H_{\text{tm}}(408\text{ K})$ kJ·mol <sup>-1</sup>	$\Delta H_{\text{vap}}(298\text{ K})$ kJ·mol <sup>-1</sup> (lit)	$\Delta H_{\text{vap}}(298\text{ K})$ kJ·mol <sup>-1</sup> (calc)
N,N-Di-n-butylamine	4214.4±74	10.987±0.18	35.04±0.62	50.1±0.6	50.2±4.5
N,N-Di-n-pentylamine	5120.2±31	12.137±0.07	42.57±0.25	61.3±2.1	60.9±4.9
N-Ethylamphetamine	5236.5±22	11.927±0.05	43.53±0.18		62.3±4.9
N,N-Di-n-hexylamine	6041.9±25	13.342±0.06	50.23±0.21	70.7±3.4	71.8±5.3
4-Benzylpiperidine	6171.3±13	12.844±0.03	51.31±0.11	74.2±1.0	73.3±5.4
N,N-Di-n-heptylamine	6950.4±12	14.533±0.03	57.78±0.10	81.3±4.9	82.5±5.8

$$\Delta H_{\text{vap}}(298.15\text{ K})/\text{kJ}\cdot\text{mol}^{-1} = (1.42\pm0.08)\Delta H_{\text{tm}}(408\text{ K}) + (0.46\pm3.56) \quad r^2 = 0.9939 \quad \text{S2)}$$

<sup>1</sup> All uncertainties represent one standard deviation.

<sup>2</sup> Vaporization enthalpies are average literature values; individual values and references are reported in Table 2.

**Table S3.** A comparison of the vapor pressures of (S) (+)-methamphetamine to N-ethylamphetamine as a function of temperature <sup>1</sup>

(S) (+)-Methamphetamine T/K		N-Ethylamphetamine p/Pa <sup>2</sup>		(S) (+)-Methamphetamine T/K		N-Ethylamphetamine p/Pa <sup>2</sup>	
298.15	39	19±11	(8.2) <sup>S1</sup>	390	5600	3900±870	
310	91	48±24		400	8200	5700±1200	
320	180	98±45		410	12000	8300±1500	
330	320	190±77		420	16000	12000±1900	
340	570	340±130		430	22000	16000±2400	
350	960	590±200		440	29000	22000±2900	
360	1600	1000±310		450	39000	30000±3400	
368.2		1500±410	(800) <sup>S2</sup>	460	50000	39000	
370	2500	1600±450		470	64000	51000	
372.2		1800±480	(2700) <sup>S3</sup>	480	81000	65000	
376.2		2100±560	(3300) <sup>S4</sup>	490	101300	82000	
378.2		2300±600	(1900) <sup>S5</sup>	500		101300	
380	3800	2500±630		507.7		120000 (101325) <sup>S1</sup>	

<sup>1</sup> N-Methylamphetamine: vapor pressures evaluated using Eq. (S1);

$$\ln(p/p^0) = 7.592 - 2119.6(T/K) - 849,290(T/K)^2 - 31,824,000(T/K)^3; \quad p^0 = 101,325\text{ Pa} \quad \text{(S3)}$$

N-ethylamphetamine: vapor pressure from  $T = (298.15\text{ to }450)\text{ K}$  evaluated by correlation;

$$\text{from } T = (460\text{ to }500)\text{ K: } \ln(p/p^0) = (8.347\pm0.01) - (2,872.4\pm3.7)(T/K) - (646,650\pm665)(T/K)^2 \quad \text{(S4)}$$

<sup>2</sup> Uncertainties are a measure of the quality of the correlation; actual uncertainties may differ.

## References

<sup>S1</sup> Estimate, EPI Suite version 4.11 (Estimation Programs Interface), The EPI Suite can be downloaded at <http://www.epa.gov/oppt/exposure/pubs/episuitd1.htm>; accessed 4/08/21.

- <sup>s2</sup> Chiavarelli, S.; Marini-Bettolo, G. B. Synthetic sympatholytic substances in the ergotamine series. II. Derivatives of benzylamine, phenethylamine, and  $\alpha$ -methylphenethylamines with amine and amide functions. *Gazzetta Chimica Italiana* **1951**, *81*, 89-97.
- <sup>s3</sup> Shiho, D.; Kanayama, K.; A new process of alkylation of amines. II. *Nippon Kagaku Kaishi* 1944, 65, 237-239.
- <sup>s4</sup> Temmler, T. H.; Keil, F.; Dobke, W.  $\beta$ -Aralkylamines. DE 767263 **1952**.
- <sup>s5</sup> Leonard, N. J.; Adamcik, J. A.; Djerassi, C.; Halpern, O. Cyclic amino acyloins and amino ketones. X. Trans-annular nitrogen-carbonyl interaction in cyclic aminoketones and optical rotatory dispersion. *J. Am. Chem. Soc.* **1958**, *80*, 4858-4862.