

Supporting Information

Modeling the thermochemistry of nitrogen-containing compounds via group additivity

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1. Experimental validation of CBS-QB3 methodology

Table S1: Training (T) and validation (V) reference data for regression of BACs: Experimental and *ab initio* calculated (with and without BACs) standard enthalpies of formation at 298 K and the corresponding deviations, expressed in kJ mol⁻¹. The experimental database entries are taken from ATcT [1], Pedley et al. [2] and the NIST database [3].

No	InChI	S_{exp}°	S_{calc}°	$S_{calc}^{\circ} - S_{exp}^{\circ}$	$C_{p,exp}^{\circ}$	$C_{p,calc}^{\circ}$	$C_{p,calc}^{\circ} - C_{p,exp}^{\circ}$
1	InChI=1S/H3N/h1H3	192.7	192.3	-0.4	37.2	35.0	-2.2
2	InChI=1S/CHN/c1-2/h1H	201.8	201.1	0.8	-	-	-
3	InChI=1S/HNO/c1-2/h1H	220.7	220.6	0.2	-	-	-
4	InChI=1S/H4N2/c1-2/h1-2H2	238.7	239.4	-0.7	-	-	-
5	InChI=1S/NO2/c2-1-3	240.0	239.8	0.2	-	-	-
6	InChI=1S/C2N2/c3-1-2-4	241.6	239.2	2.4	-	-	-
7	InChI=1S/CH5N/c1-2/h2H2,1H3	242.9	241.5	1.4	50.1	49.5	-0.6
8	InChI=1S/C2H3N/c1-2-3/h1H3	243.4	242.4	1.0	52.5	51.8	-0.7
9	InChI=1S/HNO2/c2-1-3/h(H,2,3)	249.4	248.2	1.2	0.0	0.0	0.0
10	InChI=1S/C2H5N/c1-2-3-1/h3H,1-2H2	250.6	244.1	6.5	52.6	50.7	-1.9
11	InChI=1S/C2H7N/c1-3-2/h3H,1-2H3	273.0	273.0	0.0	70.7	69.6	-1.1
12	InChI=1S/CH3NO2/c1-2(3)4/h1H3	275.0	275.3	-0.3	57.3	57.2	-0.1
13	InChI=1S/C2H7N/c1-2-3/h2-3H2,1H3	283.8	281.8	2.0	71.5	71.8	0.3
14	InChI=1S/CH3NO2/c1-4-2-3/h1H3	284.3	286.5	-2.2	63.2	64.3	1.1
15	InChI=1S/C3H9N/c1-4(2)3/h1-3H3	287.1	290.8	-3.7	-	-	-
16	InChI=1S/C3H9N/c1-3(2)4/h3H,4H2,1-2H3	312.2	311.9	0.3	97.5	95.5	-2.0
17	InChI=1S/C3H9N/c1-2-3-4/h2-4H2,1H3	325.1	322.5	2.6	91.2	95.3	4.1
18	InChI=1S/C4H7N/c1-2-3-4-5/h2-3H2,1H3	325.4	323.5	1.9	97.0	96.6	-0.4
19	InChI=1S/C4H11N/c1-4(2,3)5/h5H2,1-3H3	337.9	329.0	8.9	120.0	121.8	1.8
20	InChI=1S/C4H11N/c1-3-4(2)5/h4H,3,5H2,1-2H3	351.3	355.0	-3.7	117.2	121.3	4.1
21	InChI=1S/C4H11N/c1-3-5-4-2/h5H,3-4H2,1-2H3	352.2	346.1	6.1	115.7	123.5	7.8
22	InChI=1S/C4H11N/c1-2-3-4-5/h2-5H2,1H3	363.3	359.7	3.6	118.6	119.8	1.2
23	InChI=1S/C6H15N/c1-3-5-7-6-4-2/h7H,3-6H2,1-2H3	-	-	0.0	169.9	168.4	0.0
Mean deviation (MD)				1.3			0.8
Mean absolute deviation (MAD)				2.2			2.1
Root mean squares deviation (RMS)				3.2			2.8
Maximum absolute deviation (MAX)				8.9			7.8

2. Database for regression of GAVs

Table S2: Training (T) and validation (V) data for regression of thermodynamic group additive values: Raw and BAC-corrected standard enthalpies of formation [kJ mol⁻¹] calculated at the CBS-QB3 level of theory, molecular and intrinsic standard entropy at 298 K [J mol⁻¹ K⁻¹], total symmetry number and number of optical isomers and heat capacity values [J mol⁻¹ K⁻¹] at 300 K, 400 K, 500 K, 600 K, 800 K, 1000 K and 1500 K.

No.		InChI	$\Delta_f H^\circ$	σ	n_{opt}	S°	S_{int}°	C_p°						
								300 K	400 K	500 K	600 K	800 K	1000 K	1500 K
1	T	InChI=1S/C2H2N/c1-2-3/h1,3H	397.7	1	1	255.1	255.1	58.7	65.5	70.7	74.9	81.3	86.3	94.6
2	T	InChI=1S/C2H2N/c1-2-3/h1H2	262.2	2	1	248.0	253.8	52.5	59.8	65.8	70.7	78.6	84.6	94.2
3	T	InChI=1S/C2H3N/c1-2-3/h1H,3H2	253.1	1	1	253.6	253.6	61.3	70.4	77.5	83.2	92.3	99.5	112.1
4	T	InChI=1S/C2H3N/c1-2-3/h1H3	77.5	3	1	242.4	251.5	51.8	60.7	69.0	76.3	88.3	97.6	112.4
5	T	InChI=1S/C2H3N/c1-2-3/h3H,1H2	190.5	1	1	249.9	249.9	55.0	65.5	74.1	81.1	91.9	100.0	113.2
6	T	InChI=1S/C2H4N/c1-2-3/h1,3H2	290.8	1	1	276.7	276.7	66.7	79.0	88.8	96.4	107.8	116.3	130.6
7	T	InChI=1S/C2H4N/c1-2-3/h1-2H,3H2	315.6	1	1	270.7	270.7	63.2	76.0	86.5	95.1	108.2	117.7	132.6
8	T	InChI=1S/C2H4N/c1-2-3/h2-3H,1H2	210.7	1	1	259.8	259.8	56.5	70.2	81.9	91.4	106.0	116.6	133.4
9	T	InChI=1S/C2H4N/c1-2-3/h2H,1H3	202.8	3	1	268.8	278.0	56.9	67.5	77.6	86.6	101.2	112.3	129.7
10	T	InChI=1S/C2H4N/c1-2-3/h3H,1H3	227.5	3	1	268.6	277.7	56.6	67.5	77.7	86.6	100.9	111.7	129.0
11	T	InChI=1S/C2H4N/c1-3-2/h1-2H2	233.6	8	1	245.2	262.4	59.1	71.9	83.1	92.4	106.8	117.5	134.2
12	T	InChI=1S/C2H4N/c1-3-2/h1H,2H3	270.1	3	1	268.3	277.5	56.2	66.6	76.7	85.7	100.4	111.7	129.3
13	T	InChI=1S/C2H5N/c1-2-3/h2-3H,1H3/b3-2+	45.7	3	1	263.4	272.6	58.7	71.6	84.0	95.1	113.0	126.6	148.1
14	T	InChI=1S/C2H5N/c1-2-3/h2H,1,3H2	58.7	1	1	268.8	268.8	62.5	77.2	90.0	100.8	117.6	130.1	150.0
15	T	InChI=1S/C2H5N/c1-3-2/h1H2,2H3	80.7	3	1	266.6	275.7	60.8	73.2	85.2	96.1	113.9	127.5	148.9
16	T	InChI=1S/C2H5NO/c1-2(3)4/h1H3,3H2	-236.9	3	1	296.2	305.4	73.9	89.7	103.7	115.6	134.3	148.2	170.4
17	T	InChI=1S/C2H5NO/c1-2-3-4/h2H2,1H3	43.5	3	1	305.3	314.4	75.8	88.8	101.8	113.4	132.3	146.5	168.7
18	T	InChI=1S/C2H5NO/c1-3-2-4/h2H,1H3,3H1	-192.0	3	2	296.8	300.2	68.2	83.6	98.2	111.1	131.7	147.0	170.6
19	T	InChI=1S/C2H5NO2/c1-2-5-3-4/h2H2,1H3	-104.1	3	1	331.5	340.6	89.7	106.1	121.6	134.9	155.8	171.2	194.5
20	T	InChI=1S/C2H6N/c1-2-3/h2H,3H2,1H3	122.0	3	1	286.6	295.8	72.1	86.8	100.0	111.5	129.8	143.8	166.4
21	T	InChI=1S/C2H6N/c1-2-3/h3H,2H2,1H3	155.4	3	1	286.8	295.9	67.8	82.2	95.8	107.7	127.0	141.8	165.5
22	T	InChI=1S/C2H6N/c1-3-2/h1-2H3	161.0	18	1	281.3	305.3	60.7	75.1	89.5	102.5	123.7	139.8	164.9
23	T	InChI=1S/C2H6N/c1-3-2/h3H,1H2,2H3	156.3	6	2	285.2	294.3	72.1	86.4	99.4	110.8	129.3	143.6	166.8
24	T	InChI=1S/C2H6N2/c1-2(3)4/h1,3-4H2	51.3	2	1	280.9	286.7	89.4	114.8	134.1	147.5	164.3	175.1	192.9

25	T	InChI=1S/C2H6N2/c1-3-4-2/h1-2H3	156.2	18	1	288.8	312.9	78.4	93.8	108.9	122.4	144.6	161.5	187.8
26	T	InChI=1S/C2H6NO/c1-2-3-4/h3H,2H2,1H3	16.8	3	2	320.4	323.8	79.0	95.7	111.4	124.9	146.5	162.7	188.2
27	T	InChI=1S/C2H6NO/c1-2-3-4/h4H,2H2,1H3	42.7	3	1	311.3	320.4	80.5	97.7	113.4	126.8	147.8	163.5	188.4
28	T	InChI=1S/C2H6NO/c1-3(2)4/h1-2H3	23.7	9	1	306.2	324.5	78.5	93.6	108.7	122.4	144.6	161.5	187.8
29	T	InChI=1S/C2H7N/c1-2-3/h2-3H2,1H3	-45.3	3	1	281.8	290.9	71.8	88.6	104.2	117.7	139.6	156.4	183.7
30	T	InChI=1S/C2H7N/c1-3-2/h3H,1-2H3	-14.8	9	1	273.0	291.3	69.6	86.7	102.9	117.0	139.7	157.0	184.7
31	T	InChI=1S/C2H7NO/c1-2-3-4/h3-4H,2H2,1H3	-78.8	3	1	306.7	315.9	86.7	108.2	127.5	143.6	167.6	184.4	209.5
32	T	InChI=1S/C2H7NO/c1-3(2)4/h4H,1-2H3	-67.7	9	1	296.7	315.0	89.6	111.0	129.5	144.6	167.2	183.4	208.6
33	T	InChI=1S/C2H8N2/c1-2(3)4/h2H,3-4H2,1H3	-39.9	3	1	313.9	323.1	92.9	115.9	135.7	151.9	176.4	194.7	224.4
34	T	InChI=1S/C2H8N2/c1-2-4-3/h4H,2-3H2,1H3	70.5	3	2	316.1	319.5	97.0	118.3	136.6	152.0	176.5	195.2	225.7
35	T	InChI=1S/C2H8N2/c1-3-4-2/h3-4H,1-2H3	97.6	18	4	307.6	320.1	91.6	113.9	133.9	150.7	177.0	196.4	226.8
36	T	InChI=1S/C2H8N2/c1-4(2)3/h3H2,1-2H3	84.2	9	1	302.8	321.0	90.6	113.8	134.4	151.4	177.5	196.8	227.0
37	T	InChI=1S/C2H8N2/c1-4-2-3/h4H,2-3H2,1H3	4.1	3	2	325.3	328.6	95.3	114.5	132.5	148.2	173.5	192.8	223.9
38	T	InChI=1S/C3H10N2/c1-2-3(4)5/h3H,2,4-5H2,1H3	-58.0	3	1	351.6	360.8	117.7	145.8	170.6	191.3	223.1	246.5	284.2
39	T	InChI=1S/C3H10N2/c1-3(2)5-4/h3,5H,4H2,1-2H3	37.3	9	2	343.5	356.0	124.0	151.3	174.8	194.5	225.3	248.6	286.1
40	T	InChI=1S/C3H10N2/c1-3(4)5-2/h3,5H,4H2,1-2H3/t3-/m1/s1	-33.0	9	2	348.4	360.9	118.9	146.2	170.6	191.2	223.0	246.8	284.8
41	T	InChI=1S/C3H10N2/c1-3-5(2)4/h3-4H2,1-2H3	58.8	9	2	346.1	358.6	117.1	145.0	170.2	191.5	224.5	248.9	287.1
42	T	InChI=1S/C3H10N2/c1-5(2)3-4/h3-4H2,1-2H3	-4.3	9	1	341.6	359.8	115.0	143.1	168.7	190.4	223.9	248.5	286.7
43	T	InChI=1S/C3H3N/c1-2-3-4/h1,3-4H/b4-3+	334.7	1	1	275.5	275.5	66.4	79.1	89.5	98.0	111.1	120.7	135.9
44	T	InChI=1S/C3H4N/c1-2-3-4/h2-3H,1H2	306.2	1	1	284.0	284.0	72.6	89.8	103.4	113.9	129.0	139.6	155.8
45	T	InChI=1S/C3H4N/c1-2-3-4/h2H,1H3	228.1	3	1	294.2	303.3	68.6	82.0	94.0	104.4	120.9	133.2	152.4
46	T	InChI=1S/C3H4N/c1-2-3-4/h4H,1H3	357.7	3	1	305.6	314.7	77.7	90.0	101.1	110.8	126.4	138.2	156.7
47	T	InChI=1S/C3H4N/c1-3-4-2/h1H,2H3	392.8	3	1	297.4	306.5	73.6	86.5	97.8	107.6	123.0	134.6	152.9
48	T	InChI=1S/C3H5N/c1-2-3-4/h2,4H,1H3	171.6	3	1	288.4	297.5	76.0	90.9	104.5	116.2	135.0	149.2	171.6
49	T	InChI=1S/C3H5N/c1-2-3-4/h2-4H,1H2/b4-3-	145.5	1	1	278.0	278.0	72.5	92.2	108.8	122.2	141.7	155.3	175.6
50	T	InChI=1S/C3H5N/c1-2-3-4/h2H2,1H3	60.8	3	1	285.2	294.4	72.9	88.6	102.5	114.5	133.8	148.5	171.5
51	T	InChI=1S/C3H5N/c1-2-3-4/h4H2,1H3	219.2	1	1	308.9	308.9	82.0	96.0	108.7	119.8	137.8	151.7	174.3
52	T	InChI=1S/C3H5N/c1-3-4-2/h1,4H,2H3	262.0	3	2	297.7	301.1	80.1	94.4	107.0	117.8	135.4	148.9	170.9
53	T	InChI=1S/C3H5N/c1-3-4-2/h1H2,2H3	191.0	3	1	289.5	298.6	74.7	89.8	103.6	115.4	134.5	148.9	171.6
54	T	InChI=1S/C3H5N/c1-3-4-2/h3H,1-2H2	171.3	1	1	288.2	288.2	79.4	97.3	111.8	123.3	140.7	153.6	174.1
55	T	InChI=1S/C3H6N/c1-2-3-4/h2,4H,1,3H2	269.2	1	1	314.5	314.5	80.5	98.4	114.4	127.8	148.8	164.5	189.2
56	T	InChI=1S/C3H6N/c1-2-3-4/h2-3H,1,4H2	171.9	2	1	294.8	300.6	82.9	102.4	118.9	132.5	153.3	168.6	193.1

57	T	InChI=1S/C3H6N/c1-2-3-4/h2-4H,1H3	178.3	3	1	298.0	307.1	76.7	95.0	111.9	126.3	149.0	165.8	191.9
58	T	InChI=1S/C3H6N/c1-2-3-4/h3-4H,1-2H2/b4-3+	238.4	2	1	316.0	321.8	84.9	100.4	115.1	127.9	148.4	164.0	188.8
59	T	InChI=1S/C3H6N/c1-2-3-4/h4H,2H2,1H3	209.4	3	1	314.2	323.4	79.1	95.7	111.2	124.6	146.0	162.2	187.9
60	T	InChI=1S/C3H6N/c1-3(2)4/h1-2H3	163.5	18	1	299.1	323.1	80.2	95.7	110.6	123.9	145.5	162.0	188.0
61	T	InChI=1S/C3H6N/c1-3(2)4/h4H,1H2,2H3	174.2	6	1	299.1	314.0	77.8	97.4	114.5	128.8	150.9	167.3	192.4
62	T	InChI=1S/C3H6N/c1-3-4-2/h1,3-4H,2H3	317.5	3	2	311.3	314.7	87.7	104.8	120.1	133.2	153.8	169.0	192.3
63	T	InChI=1S/C3H6N/c1-3-4-2/h2H,3H2,1H3	244.7	3	1	312.7	321.8	80.7	97.1	112.5	125.8	147.2	163.4	188.9
64	T	InChI=1S/C3H6N/c1-3-4-2/h3-4H,1-2H2	229.4	2	1	306.9	312.7	86.3	104.2	119.7	132.7	153.1	168.4	192.4
65	T	InChI=1S/C3H6N/c1-3-4-2/h3H,1H2,2H3	199.3	3	1	295.9	305.0	78.0	96.2	112.9	127.3	149.8	166.5	192.5
66	T	InChI=1S/C3H6N/c1-3-4-2/h3H,2H2,1H3	192.4	6	1	294.4	309.3	79.1	97.2	113.8	127.9	150.3	166.9	192.8
67	T	InChI=1S/C3H6N/c1-3-4-2/h4H,1H2,2H3	295.2	3	2	318.3	321.7	79.9	96.6	112.0	125.3	146.5	162.4	187.8
68	T	InChI=1S/C3H7N/c1-2-3-4/h2-3H,4H2,1H3/b3-2+	36.8	3	1	302.8	312.0	86.8	106.3	124.0	139.2	163.0	180.7	208.7
69	T	InChI=1S/C3H7N/c1-2-3-4/h2H,1,3-4H2	65.0	1	1	304.4	304.4	88.5	109.6	127.0	141.3	163.5	180.3	207.9
70	T	InChI=1S/C3H7N/c1-2-3-4/h3-4H,2H2,1H3/b4-3+	27.5	3	1	307.3	316.4	80.1	99.5	117.6	133.4	158.5	177.5	207.3
71	T	InChI=1S/C3H7N/c1-3(2)4/h1,4H2,2H3	21.9	3	1	298.7	307.9	86.4	107.3	125.4	140.6	164.5	182.3	210.1
72	T	InChI=1S/C3H7N/c1-3(2)4/h4H,1-2H3	4.9	9	1	299.6	317.8	80.6	99.1	116.7	132.2	157.4	176.4	206.6
73	T	InChI=1S/C3H7N/c1-3-4-2/h2-3H2,1H3	55.9	3	1	298.6	307.7	84.6	104.1	121.7	137.0	161.3	179.8	208.8
74	T	InChI=1S/C3H7N/c1-3-4-2/h3-4H,1H2,2H3	61.4	3	2	298.6	301.9	83.6	103.6	121.7	137.3	162.0	180.6	210.4
75	T	InChI=1S/C3H7N/c1-3-4-2/h3H,1-2H3/b4-3+	38.3	9	1	297.5	315.8	82.1	99.8	117.1	132.6	158.0	177.3	207.5
76	T	InChI=1S/C3H7NO/c1-2-3(4)5/h2H2,1H3,4H2	-256.1	3	1	336.6	345.8	99.2	119.5	138.1	154.1	179.7	198.9	229.5
77	T	InChI=1S/C3H7NO/c1-2-3-4-5/h2-3H2,1H3	25.5	3	1	342.4	351.5	96.2	117.0	136.1	152.6	178.8	198.2	228.5
78	T	InChI=1S/C3H7NO/c1-3(2)4-5/h3H,1-2H3	11.2	3	1	333.2	342.3	98.5	118.1	136.3	152.2	177.9	197.3	227.7
79	T	InChI=1S/C3H7NO/c1-3(5)4-2/h1-2H3,4H1	-237.2	9	2	327.2	339.7	89.2	110.7	130.8	148.3	176.1	196.7	228.9
80	T	InChI=1S/C3H7NO/c1-4(2)3-5/h3H,1-2H3	-196.9	9	1	324.4	342.6	93.4	112.6	131.6	148.7	176.7	197.7	230.2
81	T	InChI=1S/C3H7NO2/c1-2-3-4(5)6/h2-3H2,1H3	-132.6	6	1	354.9	369.8	103.2	128.0	150.2	169.0	198.0	219.1	251.3
82	T	InChI=1S/C3H7NO2/c1-2-3-6-4-5/h2-3H2,1H3	-122.9	3	1	359.1	368.2	108.9	132.9	154.6	172.9	201.5	222.3	254.0
83	T	InChI=1S/C3H7NO2/c1-3(2)4(5)6/h3H,1-2H3	-147.2	18	1	346.8	370.8	104.9	129.4	151.2	169.6	198.1	219.0	250.9
84	T	InChI=1S/C3H7NO2/c1-3(2)6-4-5/h3H,1-2H3	-139.4	9	1	348.4	366.6	116.5	141.2	161.7	178.4	204.3	223.4	253.3
85	T	InChI=1S/C3H8N/c1-2-3-4/h1-4H2	143.1	2	1	335.0	340.7	93.0	114.2	133.1	149.2	174.4	193.5	224.4
86	T	InChI=1S/C3H8N/c1-2-3-4/h2H,3-4H2,1H3	133.1	3	1	334.5	343.6	92.0	111.7	130.1	146.2	172.0	191.8	223.7
87	T	InChI=1S/C3H8N/c1-2-3-4/h3H,2,4H2,1H3	104.5	3	1	325.9	335.0	93.4	114.7	133.5	149.6	174.9	194.2	225.1
88	T	InChI=1S/C3H8N/c1-2-3-4/h4H,2-3H2,1H3	140.5	3	1	327.2	336.3	90.6	111.1	130.2	146.8	173.3	193.3	225.0

89	T	InChI=1S/C3H8N/c1-3(2)4/h3-4H,1-2H3	125.2	9	1	318.5	336.7	91.6	112.9	131.9	148.1	173.9	193.5	224.9
90	T	InChI=1S/C3H8N/c1-3(2)4/h4H2,1-2H3	77.5	18	1	316.6	340.6	97.0	115.8	133.2	148.5	173.6	193.0	224.5
91	T	InChI=1S/C3H8N/c1-3-4-2/h3H2,1-2H3	134.9	9	2	323.0	335.5	88.1	107.8	126.9	143.8	171.2	192.0	224.7
92	T	InChI=1S/C3H8N/c1-3-4-2/h4H,1,3H2,2H3	169.4	6	2	325.6	334.7	98.3	117.5	135.4	150.9	176.0	195.2	226.0
93	T	InChI=1S/C3H8N/c1-3-4-2/h4H,2-3H2,1H3	131.8	9	2	324.4	336.9	96.8	116.8	134.9	150.4	175.5	194.8	225.8
94	T	InChI=1S/C3H8N2/c1-2-3(4)5/h2-3H,1,4-5H2	74.2	1	1	338.3	338.3	111.1	136.7	157.5	174.0	198.7	217.2	247.6
95	T	InChI=1S/C3H8N2/c1-3(4)5-2/h5H,1,4H2,2H3	54.6	3	2	322.4	325.7	108.3	138.9	164.6	184.4	211.3	228.6	254.4
96	T	InChI=1S/C3H8N2/c1-3-5-4-2/h3H2,1-2H3	131.1	9	1	334.6	352.9	101.1	122.7	143.1	161.2	190.4	212.4	247.0
97	T	InChI=1S/C3H8NO/c1-3(2)4-5/h3,5H,1-2H3	11.9	9	1	341.0	359.2	107.4	130.8	151.3	168.5	195.5	215.8	248.0
98	T	InChI=1S/C3H8NO/c1-3(2)4-5/h3-4H,1-2H3	-16.3	9	2	349.8	362.3	103.9	126.4	146.9	164.6	192.8	214.1	247.5
99	T	InChI=1S/C3H8NO/c1-3-4(2)5/h3H2,1-2H3	-3.1	9	2	350.3	362.8	102.0	123.1	143.5	161.6	190.8	212.8	247.2
100	T	InChI=1S/C3H9N/c1-2-3-4/h2-4H2,1H3	-63.3	3	1	322.5	331.7	95.3	117.9	138.8	156.8	185.8	207.8	243.2
101	T	InChI=1S/C3H9N/c1-3(2)4/h3H,4H2,1-2H3	-80.7	9	1	311.9	330.2	95.5	119.5	140.8	158.7	187.1	208.7	243.6
102	T	InChI=1S/C3H9N/c1-3-4-2/h4H,3H2,1-2H3	-40.7	9	2	315.0	327.5	96.4	118.4	139.0	157.1	186.5	208.9	244.5
103	T	InChI=1S/C3H9N/c1-4(2)3/h1-3H3	-24.3	81	1	290.8	327.3	91.3	115.5	138.2	157.7	188.4	211.1	246.4
104	T	InChI=1S/C3H9NO/c1-3(2)4-5/h3-5H,1-2H3	-112.2	9	1	334.3	352.6	112.7	140.0	164.5	184.8	215.4	236.9	269.5
105	T	InChI=1S/C3H9NO/c1-3-4(2)5/h5H,3H2,1-2H3	-94.6	9	2	336.5	349.0	118.0	144.9	168.0	186.9	215.8	236.8	269.3
106	T	InChI=1S/C4H10N/c1-2-3-4-5/h2H,3-5H2,1H3	112.8	3	1	374.6	383.8	113.1	139.3	163.7	184.7	218.1	243.3	283.3
107	T	InChI=1S/C4H10N/c1-2-3-4-5/h3H,2,4-5H2,1H3	116.0	3	1	377.9	387.0	110.9	138.1	162.7	183.7	217.0	242.2	282.5
108	T	InChI=1S/C4H10N/c1-2-3-4-5/h4H,2-3,5H2,1H3	86.1	3	1	364.5	373.6	118.0	145.0	169.1	189.7	222.1	246.6	285.4
109	T	InChI=1S/C4H10N/c1-3-4(2)5/h3,5H2,1-2H3	61.4	9	1	364.1	382.3	115.9	142.1	165.8	186.3	219.1	244.0	283.7
110	T	InChI=1S/C4H10N/c1-3-5-4-2/h3,5H,4H2,1-2H3	99.1	9	2	363.9	376.4	125.4	147.9	169.9	189.5	221.6	246.1	285.3
111	T	InChI=1S/C4H10N/c1-3-5-4-2/h3-4H2,1-2H3	108.8	18	1	355.2	379.2	114.7	140.4	164.4	185.3	219.0	244.6	284.8
112	T	InChI=1S/C4H10N/c1-3-5-4-2/h5H,1,3-4H2,2H3	143.3	6	2	364.2	373.4	124.6	148.5	170.9	190.6	222.6	246.9	285.8
113	T	InChI=1S/C4H10N/c1-4(2)3-5/h4-5H,3H2,1-2H3	108.2	9	1	352.0	370.3	117.5	144.3	168.7	189.4	222.1	246.7	285.6
114	T	InChI=1S/C4H10N2/c1-3-4(5)6-2/h3-4,6H,1,5H2,2H3/t4-/m1/s1	75.5	3	2	364.6	368.0	138.0	174.5	203.6	225.4	255.6	277.0	311.6
115	T	InChI=1S/C4H10N2/c1-3-5-6-4-2/h3-4H2,1-2H3	105.7	18	1	372.5	396.5	124.0	151.7	177.4	199.9	236.1	263.4	306.1
116	T	InChI=1S/C4H11N/c1-2-3-4-5/h2-5H2,1H3	-81.3	3	1	359.8	368.9	119.8	147.4	173.3	195.8	231.9	259.3	302.9
117	T	InChI=1S/C4H11N/c1-3-4(2)5/h4H,3,5H2,1-2H3/t4-/m1/s1	-95.7	9	2	355.0	367.5	121.3	150.2	176.3	198.5	233.8	260.5	303.4
118	T	InChI=1S/C4H11N/c1-3-5-4-2/h5H,3-4H2,1-2H3	-63.2	9	1	346.1	364.4	123.5	150.3	175.5	197.6	233.5	261.0	304.4
119	T	InChI=1S/C4H11N/c1-4(2)3-5/h4H,3,5H2,1-2H3	-90.4	9	1	349.7	368.0	119.3	148.4	175.0	197.6	233.5	260.5	303.5
120	T	InChI=1S/C4H11N/c1-4(2)5-3/h4-5H,1-3H3	-72.7	27	2	344.6	366.2	119.6	148.6	174.9	197.5	233.6	260.9	304.2

121	T	InChI=1S/C4H11N/c1-4(2,3)5/h5H2,1-3H3	-115.7	81	1	329.0	365.6	121.8	152.8	179.5	201.6	236.0	262.1	304.0
122	T	InChI=1S/C4H11N/c1-4-5(2)3/h4H2,1-3H3	-46.9	27	1	340.4	367.8	115.2	144.7	172.1	195.9	233.6	261.8	305.6
123	T	InChI=1S/C4H11NO/c1-3-5(6)4-2/h6H,3-4H2,1-2H3	-121.3	9	1	363.2	381.5	146.7	179.1	206.5	229.3	264.4	290.2	330.2
124	T	InChI=1S/C4H12N2/c1-4-6(3)5-2/h5H,4H2,1-3H3	61.7	27	4	375.3	391.2	138.1	170.6	200.5	226.4	267.7	298.8	347.4
125	T	InChI=1S/C4H3N/c1-2-3-4-5/h1H3	328.1	3	1	289.7	298.8	80.6	93.5	104.6	114.1	129.5	141.0	158.8
126	T	InChI=1S/C4H4N/c1-2-3-4-5/h2-3H,1H2	292.5	1	1	305.4	305.4	83.2	101.0	115.9	128.0	146.3	159.5	179.8
127	T	InChI=1S/C4H4N/c1-3-5-4-2/h1,4H,2H2	459.3	1	1	304.0	304.0	91.4	110.2	124.5	135.7	152.3	164.2	181.9
128	T	InChI=1S/C4H5N/c1-2-3-4-5/h2-3H,1H3/b3-2+	157.8	3	1	308.0	317.2	86.3	103.7	119.3	132.7	154.0	170.0	194.6
129	T	InChI=1S/C4H5N/c1-2-3-4-5/h2H,1,3H2	174.3	1	1	318.6	318.6	85.3	103.7	119.7	133.3	154.5	170.3	194.7
130	T	InChI=1S/C4H5N/c1-2-3-4-5/h4-5H,1H3/b5-4+	290.3	3	1	323.1	332.2	88.4	105.7	121.6	135.2	156.9	173.1	198.1
131	T	InChI=1S/C4H5N/c1-3-5-4-2/h1,4-5H,2H2	345.3	1	2	330.0	324.3	97.4	115.2	130.1	142.4	161.3	175.2	197.2
132	T	InChI=1S/C4H5N/c1-4(2)3-5/h1H2,2H3	158.5	3	1	307.0	316.2	86.7	104.6	120.2	133.4	154.4	170.1	194.6
133	T	InChI=1S/C4H6N/c1-2-3-4-5/h3H,2H2,1H3	209.6	3	1	335.0	344.2	90.1	110.2	127.9	142.9	166.6	184.2	211.5
134	T	InChI=1S/C4H6N/c1-3-4-5-2/h3H,2H2,1H3	343.6	3	1	331.3	340.4	96.9	116.9	134.5	149.4	172.4	189.2	214.8
135	T	InChI=1S/C4H6N/c1-3-5-4-2/h1H,4H2,2H3	365.7	3	1	336.7	345.8	95.5	114.9	131.9	146.3	168.9	185.8	212.2
136	T	InChI=1S/C4H6N/c1-3-5-4-2/h3-4H,1-2H2	262.6	2	1	299.1	304.8	91.3	118.5	142.7	162.2	189.1	205.4	225.7
137	T	InChI=1S/C4H6N/c1-3-5-4-2/h4H,1H2,2H3	324.9	3	1	330.2	339.3	95.7	116.2	134.1	149.2	172.7	189.8	215.7
138	T	InChI=1S/C4H6N/c1-4(2)3-5/h1-2H3	190.0	18	1	326.6	350.6	88.7	107.2	124.5	139.7	164.2	182.5	210.7
139	T	InChI=1S/C4H7N/c1-2-3-4-5/h2,5H2,1H3	201.4	3	1	331.7	340.8	102.8	124.1	142.7	158.6	183.8	202.9	233.6
140	T	InChI=1S/C4H7N/c1-2-3-4-5/h2-3H2,1H3	39.0	3	1	323.5	332.6	96.6	118.4	137.9	154.4	180.7	200.4	231.3
141	T	InChI=1S/C4H7N/c1-2-3-4-5/h2-5H,1H3/b3-2+,5-4-	121.4	3	1	314.3	323.4	95.9	118.8	139.1	156.3	183.1	202.7	232.8
142	T	InChI=1S/C4H7N/c1-3-4-5-2/h3-4H,1H2,2H3/b5-4-	136.7	3	1	312.4	321.5	96.3	120.6	141.9	159.6	186.6	206.0	235.1
143	T	InChI=1S/C4H7N/c1-3-4-5-2/h3-4H,2H2,1H3/b4-3+	140.8	3	1	312.5	321.6	96.9	122.0	143.7	161.3	187.1	205.4	233.9
144	T	InChI=1S/C4H7N/c1-3-5-4-2/h1,4H2,2H3	164.2	3	1	329.2	338.3	96.6	118.6	138.1	154.7	180.8	200.3	231.1
145	T	InChI=1S/C4H7N/c1-3-5-4-2/h1,5H,4H2,2H3	234.6	3	2	339.2	342.5	102.8	124.0	142.3	157.7	182.2	200.8	230.6
146	T	InChI=1S/C4H7N/c1-3-5-4-2/h3-4H,1H2,2H3/b5-4-	127.6	3	1	316.4	325.5	99.8	123.3	143.1	159.3	184.4	203.1	232.5
147	T	InChI=1S/C4H7N/c1-3-5-4-2/h3-5H,1-2H2	146.6	2	1	319.1	324.9	108.7	131.2	150.1	166.1	191.2	209.8	238.2
148	T	InChI=1S/C4H7N/c1-4(2)3-5/h4H,1-2H3	34.9	9	1	315.3	333.5	97.3	119.4	138.7	155.1	181.0	200.4	231.2
149	T	InChI=1S/C4H7N/c1-4(2)5-3/h1,3H2,2H3	139.6	3	1	322.5	331.6	95.6	118.3	138.2	155.0	181.3	200.9	231.4
150	T	InChI=1S/C4H8N/c1-3-4(2)5/h3H,1,5H2,2H3	128.6	6	1	329.5	344.4	107.0	131.6	153.0	171.1	199.3	220.3	253.1
151	T	InChI=1S/C4H8N/c1-3-4-5-2/h3-5H,1H2,2H3	171.7	6	2	335.6	344.7	102.4	126.8	148.9	167.6	197.1	219.1	253.7
152	T	InChI=1S/C4H8N/c1-3-4-5-2/h4H,2-3H2,1H3	174.0	6	1	346.5	361.4	101.7	126.0	148.0	166.9	196.8	218.8	252.4

153	T	InChI=1S/C4H8N/c1-3-5-4-2/h5H,1,4H2,2H3	268.7	3	2	348.5	351.9	106.7	131.7	153.5	171.3	198.2	218.0	249.3
154	T	InChI=1S/C4H8N/c1-4(2)3-5/h3,5H,1-2H3	134.7	18	1	325.7	349.8	98.4	121.8	143.8	162.8	193.0	215.5	250.4
155	T	InChI=1S/C4H8N/c1-4(2)3-5/h3H,1,5H2,2H3	139.2	6	1	332.2	347.1	104.7	130.1	152.1	170.4	198.8	219.8	252.7
156	T	InChI=1S/C4H8N/c1-4(2)3-5/h4-5H,1-2H3	184.2	9	1	338.1	356.4	101.7	125.7	146.9	164.8	193.0	214.2	247.6
157	T	InChI=1S/C4H8N/c1-4(2)5-3/h1H2,2-3H3	169.1	9	1	333.1	351.4	95.4	120.8	143.6	163.0	193.4	215.8	250.7
158	T	InChI=1S/C4H8N/c1-4(2)5-3/h3H2,1-2H3	156.7	36	1	335.9	365.7	101.6	124.8	146.3	164.9	194.6	216.7	251.2
159	T	InChI=1S/C4H8N/c1-4-5(2)3/h1H2,2-3H3	289.7	9	1	345.7	364.0	103.4	126.1	147.9	166.7	196.1	217.3	249.8
160	T	InChI=1S/C4H9N/c1-2-3-4-5/h2-3H,4-5H2,1H3/b3-2+	34.7	3	1	346.6	355.7	109.7	134.9	157.3	176.3	206.4	229.3	266.1
161	T	InChI=1S/C4H9N/c1-2-3-4-5/h3-4H,2,5H2,1H3/b4-3+	18.2	3	1	340.2	349.4	109.9	136.0	159.4	179.2	210.2	233.1	268.9
162	T	InChI=1S/C4H9N/c1-3-4(2)5/h2-3,5H2,1H3	5.4	3	1	338.0	347.1	108.1	135.7	159.7	179.8	210.9	233.8	269.5
163	T	InChI=1S/C4H9N/c1-3-4(2)5/h3-4H,1,5H2,2H3/t4-/m0/s1	30.7	3	2	339.2	342.6	113.1	141.0	164.0	182.7	211.4	232.9	267.8
164	T	InChI=1S/C4H9N/c1-3-4-5-2/h3,5H,1,4H2,2H3	69.4	3	2	337.9	341.3	110.9	137.6	160.8	180.1	210.3	232.8	268.6
165	T	InChI=1S/C4H9N/c1-3-4-5-2/h4H,3H2,1-2H3/b5-4+	20.0	9	1	340.4	358.6	104.2	127.7	150.2	170.3	202.9	227.7	266.5
166	T	InChI=1S/C4H9N/c1-3-5-4-2/h3,5H,1,4H2,2H3	36.6	3	2	343.0	346.3	110.4	135.5	158.7	178.8	210.9	234.8	271.6
167	T	InChI=1S/C4H9N/c1-3-5-4-2/h3H,4H2,1-2H3/b5-3+	12.3	9	1	334.2	352.4	105.1	130.4	153.5	173.5	205.5	229.7	267.4
168	T	InChI=1S/C4H9N/c1-4(2)3-5/h1,3,5H2,2H3	29.7	3	1	341.7	350.9	114.0	137.1	158.5	177.1	206.9	229.7	266.3
169	T	InChI=1S/C4H9N/c1-4(2)3-5/h3-5H,1-2H3/b5-3+	1.6	9	1	335.1	353.3	104.5	130.0	153.2	173.1	204.9	228.9	266.6
170	T	InChI=1S/C4H9N/c1-4(2)3-5/h3H,5H2,1-2H3	5.6	9	1	336.7	355.0	107.8	133.3	156.2	175.7	206.6	229.7	266.6
171	T	InChI=1S/C4H9N/c1-4(2)5-3/h1-3H3	10.1	27	1	336.2	363.6	97.8	122.5	146.0	166.8	200.3	225.7	265.2
172	T	InChI=1S/C4H9N/c1-4(2)5-3/h5H,1H2,2-3H3	23.4	9	2	332.1	344.6	109.9	136.7	160.2	180.1	211.6	235.0	271.1
173	T	InChI=1S/C4H9N/c1-4-5(2)3/h4H,1H2,2-3H3	58.8	9	1	336.2	354.4	104.7	129.5	153.0	173.8	207.2	232.3	270.5
174	T	InChI=1S/C4H9NO/c1-2-3-4(5)6/h2-3H2,1H3,5H2	-275.3	3	1	371.9	381.1	123.8	150.9	175.0	195.5	227.9	251.9	289.9
175	T	InChI=1S/C4H9NO/c1-3(2)4(5)6/h3H,1-2H3,5H2	-281.0	9	1	364.8	383.0	125.6	151.9	175.4	195.5	227.3	251.2	289.2
176	T	InChI=1S/C4H9NO/c1-3-4(2)5-6/h4H,3H2,1-2H3/t4-/m1/s1	-7.2	9	2	375.7	388.2	126.1	150.4	173.2	193.2	225.4	249.6	287.7
177	T	InChI=1S/C4H9NO/c1-3-5-4(2)6/h3H2,1-2H3,5H1	-264.1	9	2	370.3	382.8	112.2	141.0	167.0	189.3	224.2	249.8	289.5
178	T	InChI=1S/C4H9NO/c1-4(2)3-5-6/h4H,3H2,1-2H3	-1.2	9	1	368.2	386.4	121.3	148.6	173.2	194.1	226.8	251.1	288.7
179	T	InChI=1S/C4H9NO/c1-4(6)5(2)3/h1-3H3	-231.1	27	1	358.6	386.0	112.5	137.8	162.4	184.4	220.1	246.8	288.1
180	T	InChI=1S/C4H9NO2/c1-2-3-4-5(6)7/h2-4H2,1H3	-151.5	6	1	392.6	407.5	128.8	158.5	185.4	208.4	244.4	270.7	310.8
181	T	InChI=1S/C4H9NO2/c1-3-4(2)5(6)7/h4H,3H2,1-2H3/t4-/m1/s1	-168.5	18	2	387.3	405.6	132.9	162.3	188.6	211.0	245.9	271.6	310.9
182	T	InChI=1S/C4H9NO2/c1-3-4(2)7-5-6/h4H,3H2,1-2H3/t4-/m1/s1	-159.7	9	2	391.3	403.8	142.3	172.6	198.4	219.7	252.4	276.3	313.6
183	T	InChI=1S/C4H9NO2/c1-4(2)3-5(6)7/h4H,3H2,1-2H3	-161.0	18	1	384.8	408.8	129.3	159.9	187.2	210.1	245.6	271.5	310.9
184	T	InChI=1S/C4H9NO2/c1-4(2)3-7-5-6/h4H,3H2,1-2H3	-150.2	9	1	389.0	407.2	134.7	164.8	191.9	214.7	249.9	275.5	314.5

185	T	InChI=1S/C5H10N/c1-3-4-5(2)6/h3-4H,6H2,1-2H3	101.8	9	1	371.7	390.0	127.5	156.7	183.4	206.4	242.7	269.6	311.5
186	T	InChI=1S/C5H10N/c1-3-5(2)4-6/h4,6H,3H2,1-2H3	117.3	9	1	369.4	387.6	121.4	151.8	179.4	202.9	239.9	267.4	310.1
187	T	InChI=1S/C5H10N/c1-4-5(2)6-3/h4,6H,1H2,2-3H3	138.6	18	2	370.4	388.6	126.1	155.4	182.0	204.9	241.2	268.3	310.7
188	T	InChI=1S/C5H10N/c1-4-6-5(2)3/h2,4H2,1,3H3	143.7	18	1	367.4	391.5	123.6	154.3	182.0	205.6	242.8	270.2	312.5
189	T	InChI=1S/C5H10N/c1-4-6-5(2)3/h4H,1-3H3	117.5	54	1	364.1	397.2	121.8	151.4	179.9	204.9	244.0	272.0	312.8
190	T	InChI=1S/C5H10N/c1-5(2)4-6-3/h4H,1-3H3	125.2	54	1	360.4	393.6	120.6	148.2	175.0	198.7	236.9	265.5	309.6
191	T	InChI=1S/C5H11N/c1-2-3-4-5-6/h3-4H,2,5-6H2,1H3/b4-3+	16.8	3	1	383.3	392.5	135.5	166.8	194.1	217.1	253.7	281.4	325.9
192	T	InChI=1S/C5H11N/c1-3-4-5-6-2/h3-4,6H,5H2,1-2H3/b4-3+	38.9	9	2	373.1	385.6	135.0	165.8	193.5	217.2	254.7	282.8	327.4
193	T	InChI=1S/C5H11N/c1-3-5(2)4-6/h4-6H,3H2,1-2H3	-15.9	9	2	377.3	389.8	132.3	162.2	189.8	213.8	252.1	281.0	326.5
194	T	InChI=1S/C5H11N/c1-3-5(2)4-6/h4H,3,6H2,1-2H3/b5-4-	-11.7	9	1	374.3	392.5	130.4	162.1	190.6	214.8	252.9	281.3	326.2
195	T	InChI=1S/C5H11N/c1-3-5-6-4-2/h3,6H,1,4-5H2,2H3	43.1	3	2	375.9	379.3	138.1	169.5	197.1	220.5	257.2	284.8	328.5
196	T	InChI=1S/C5H11N/c1-4(2)5(3)6/h5H,1,6H2,2-3H3/t5-/m1/s1	-2.8	9	2	374.0	386.5	134.9	168.5	196.9	220.2	256.3	283.4	326.6
197	T	InChI=1S/C5H11N/c1-4-5(2)6-3/h4-6H,1H2,2-3H3/t5-/m0/s1	38.9	9	4	374.9	381.6	133.7	166.7	195.7	219.8	257.2	284.9	328.4
198	T	InChI=1S/C5H11N/c1-4-5(2)6-3/h4H2,1-3H3/b6-5+	-10.1	27	1	376.9	404.3	122.7	152.0	180.3	205.4	246.0	276.7	324.5
199	T	InChI=1S/C5H11N/c1-4-5(2,3)6/h4H,1,6H2,2-3H3	-3.3	9	1	365.0	383.2	137.2	169.9	198.0	221.2	257.1	283.9	327.1
200	T	InChI=1S/C5H11N/c1-4-6(3)5-2/h4H,1,5H2,2-3H3	34.8	9	2	366.6	379.1	131.9	162.7	190.9	215.4	254.4	283.8	329.9
201	T	InChI=1S/C5H11N/c1-4-6-5(2)3/h4H2,1-3H3	-19.4	27	1	374.6	402.0	121.5	152.7	182.1	207.7	248.8	279.5	326.7
202	T	InChI=1S/C5H11N/c1-4-6-5(2)3/h6H,2,4H2,1,3H3	-2.1	9	2	368.7	381.2	136.6	168.5	196.8	220.9	259.2	287.8	331.8
203	T	InChI=1S/C5H11N/c1-5(2)4-6-3/h4,6H,1-3H3	13.7	27	2	370.4	392.1	129.4	161.0	190.1	215.1	254.1	282.8	327.6
204	T	InChI=1S/C5H11NO/c1-3-5(4-2)6-7/h5H,3-4H2,1-2H3	-26.3	9	1	402.3	420.5	156.8	185.8	212.5	235.9	273.8	302.5	347.9
205	T	InChI=1S/C5H11NO/c1-4-5(7)6(2)3/h4H2,1-3H3	-250.1	27	1	391.5	418.9	139.6	169.3	198.4	224.5	267.1	299.1	348.5
206	T	InChI=1S/C5H11NO/c1-5(2,3)4(6)7/h1-3H3,6H2	-310.7	81	1	381.0	417.5	146.2	181.4	211.7	236.8	275.6	304.3	349.3
207	T	InChI=1S/C5H11NO2/c1-3-5(4-2)6(7)8/h5H,3-4H2,1-2H3	-190.2	18	1	414.7	438.7	159.9	194.6	226.1	252.9	294.6	325.0	371.5
208	T	InChI=1S/C5H11NO2/c1-5(2,3)4-6(7)8/h4H2,1-3H3	-191.4	16	1	400.2	442.5	155.3	192.3	225.0	252.2	294.1	324.5	370.6
209	T	InChI=1S/C5H12N/c1-4-5(2)6-3/h6H,4H2,1-3H3	76.1	27	1	391.0	418.4	140.2	170.8	199.8	225.2	265.8	296.4	344.4
210	T	InChI=1S/C5H12N2/c1-3-5-7-6-4-2/h3-5H2,1-2H3	86.7	9	1	418.7	436.9	147.1	181.3	212.7	239.8	283.0	315.4	365.8
211	T	InChI=1S/C5H13N/c1-2-3-4-5-6/h2-6H2,1H3	-99.5	3	1	397.3	406.4	145.3	177.6	208.3	235.1	278.2	310.8	362.6
212	T	InChI=1S/C5H13N/c1-3-4-5(2)6/h5H,3-4,6H2,1-2H3/t5-/m1/s1	-116.0	9	2	392.4	404.9	146.0	180.8	211.8	238.3	280.4	312.4	363.2
213	T	InChI=1S/C5H13N/c1-3-5(6)4-2/h5H,3-4,6H2,1-2H3	-113.1	9	1	386.5	404.8	147.9	181.1	211.6	238.1	280.2	312.2	363.1
214	T	InChI=1S/C5H13N/c1-4-5(2,3)6/h4,6H2,1-3H3	-130.5	27	1	375.5	402.9	144.4	181.0	213.1	239.9	281.9	313.3	363.5
215	T	InChI=1S/C5H13N/c1-4-6-5(2)3/h5-6H,4H2,1-3H3	-98.6	27	2	382.6	404.2	145.1	180.2	211.5	238.4	281.3	313.6	364.6
216	T	InChI=1S/C5H13N/c1-5(2,3)6-4/h6H,1-4H3	-102.7	24	2	359.9	399.8	142.2	179.0	211.3	238.4	281.0	312.9	363.6

217	T	InChI=1S/C5H4N/c1-3-5-6-4-2/h2H,1H3	625.7	3	1	354.1	363.2	106.6	123.9	138.1	150.0	168.6	182.4	203.5
218	T	InChI=1S/C5H6N/c1-2-3-4-5-6/h2-4H,1H3	257.9	3	1	343.8	353.0	104.6	127.0	146.9	163.7	189.8	209.0	238.4
219	T	InChI=1S/C5H6N/c1-3-5(2)4-6/h3H,2H2,1H3	276.1	6	1	334.7	349.6	106.2	129.4	149.2	165.6	191.0	209.6	238.5
220	T	InChI=1S/C5H6N/c1-3-5-6-4-2/h4H,2H2,1H3	421.1	3	1	352.8	361.9	112.1	135.8	155.7	172.3	197.9	216.4	243.9
221	T	InChI=1S/C5H6N/c1-4-6-5(2)3/h1H,2H2,3H3	421.3	3	1	353.2	362.3	125.1	148.8	167.5	182.6	205.8	222.7	248.4
222	T	InChI=1S/C5H7N/c1-2-3-4-5-6/h2-3H,4H2,1H3/b3-2+	142.1	3	1	354.7	363.8	108.3	131.4	152.2	170.2	198.9	220.3	253.5
223	T	InChI=1S/C5H7N/c1-3-4-5-6-2/h5H,1-2H3/b6-5+	284.2	9	1	365.5	383.7	108.7	131.4	152.6	171.1	200.8	223.0	257.0
224	T	InChI=1S/C5H7N/c1-3-5(2)4-6/h2-3H2,1H3	138.6	3	1	346.7	355.9	109.4	133.8	154.9	172.7	200.7	221.5	254.0
225	T	InChI=1S/C5H7N/c1-3-5(2)4-6/h3H,1-2H3/b5-3-	121.9	9	1	341.4	359.7	109.2	131.5	151.9	169.6	198.3	219.8	253.2
226	T	InChI=1S/C5H7N/c1-3-5-6-4-2/h2-3,5-6H,1H3/b5-3+	321.2	3	2	366.0	369.4	118.5	141.6	161.8	178.8	205.3	224.9	255.5
227	T	InChI=1S/C5H7N/c1-4-6-5(2)3/h1,6H,2H2,3H3	306.1	3	2	356.8	360.2	119.3	143.5	163.9	180.9	207.4	226.9	257.2
228	T	InChI=1S/C5H7N/c1-5(2)3-4-6/h1,3H2,2H3	137.1	3	1	347.8	356.9	108.7	132.7	153.7	171.5	199.8	220.9	253.7
229	T	InChI=1S/C5H7N/c1-5(2)3-4-6/h3H,1-2H3	116.1	9	1	341.6	359.8	109.5	131.9	152.3	170.1	198.6	220.0	253.3
230	T	InChI=1S/C5H8N/c1-3-5(2)4-6/h3H2,1-2H3	170.1	9	1	373.4	391.7	110.8	135.7	158.6	178.3	209.9	233.5	270.0
231	T	InChI=1S/C5H8N/c1-3-5-6-4-2/h3-4H,1-2H3	302.6	9	1	369.9	388.1	114.9	140.6	163.9	184.0	215.6	238.8	273.9
232	T	InChI=1S/C5H8N/c1-4-6-5(2)3/h1,5H,2-3H3	333.1	3	1	373.7	382.8	123.2	148.1	169.8	188.1	216.7	238.2	271.9
233	T	InChI=1S/C5H8N/c1-4-6-5(2)3/h4H,1-2H2,3H3	234.0	12	1	329.8	350.5	121.7	152.8	178.5	199.7	231.3	252.6	281.8
234	T	InChI=1S/C5H8N/c1-5(2)3-4-6/h5-6H,1-2H3	313.4	9	1	368.2	386.4	123.2	148.9	171.3	190.1	219.5	241.3	275.7
235	T	InChI=1S/C5H9N/c1-3-5(2)4-6/h5H,3H2,1-2H3/t5-/m0/s1	14.4	9	2	359.5	372.0	122.9	149.9	174.2	194.9	227.7	252.3	291.0
236	T	InChI=1S/C5H9N/c1-3-5(6)4-2/h3-5H,1-2,6H2	142.2	1	1	361.4	361.4	130.9	159.6	183.3	202.6	232.5	254.9	291.1
237	T	InChI=1S/C5H9N/c1-3-5-6-4-2/h3,5H,1,4H2,2H3/b6-5-	110.5	3	1	349.3	358.4	119.6	151.3	178.4	200.6	234.1	258.3	294.9
238	T	InChI=1S/C5H9N/c1-3-5-6-4-2/h3-6H,2H2,1H3/b5-3+	124.0	3	2	364.7	368.1	129.9	157.0	181.0	201.7	234.6	258.9	296.2
239	T	InChI=1S/C5H9N/c1-4-6-5(2)3/h1,5-6H,2-3H3	199.3	9	2	358.9	371.4	128.5	156.1	179.6	199.2	230.0	253.3	290.6
240	T	InChI=1S/C5H9N/c1-4-6-5(2)3/h4,6H,1-2H2,3H3	111.2	3	2	357.4	360.8	126.3	155.4	181.0	202.3	235.0	258.7	294.9
241	T	InChI=1S/C5H9N/c1-4-6-5(2)3/h4H,2H2,1,3H3/b6-4-	94.7	9	1	357.7	375.9	119.7	146.8	171.3	192.3	225.8	250.9	290.1
242	T	InChI=1S/C5H9N/c1-5(2)3-4-6/h3-4,6H,1-2H3/b6-4-	84.1	9	1	347.7	366.0	120.8	148.0	172.7	194.0	227.9	253.1	291.8
243	T	InChI=1S/C5H9N/c1-5(2,3)4-6/h1-3H3	2.9	81	1	331.8	368.3	123.7	152.4	177.0	197.6	229.6	253.6	291.5
244	T	InChI=1S/C6H11N/c1-3-5-6(7)4-2/h3-6H,2,7H2,1H3/b5-3-/t6-/m0/s1	117.8	3	2	402.5	405.9	150.7	184.6	214.1	238.7	276.9	305.2	350.0
245	T	InChI=1S/C6H11N/c1-3-6(2)4-5-7/h4-5,7H,3H2,1-2H3/b6-4+,7-5+	67.3	9	1	383.7	401.9	141.6	175.9	207.0	233.5	274.9	305.3	351.8
246	T	InChI=1S/C6H11N/c1-3-6(4-2)5-7/h6H,3-4H2,1-2H3	-6.0	9	1	390.3	408.5	149.2	181.0	210.0	234.9	274.6	304.3	350.8
247	T	InChI=1S/C6H11N/c1-4-6(2,3)5-7/h4H2,1-3H3	-16.2	27	1	380.5	407.9	147.5	182.0	211.9	236.9	276.1	305.3	351.2
248	T	InChI=1S/C6H11N/c1-4-6(5-2)7-3/h4-7H,1-2H2,3H3	147.1	3	1	385.1	394.2	150.9	189.0	220.2	245.1	282.5	309.8	353.0

249	T	InChI=1S/C6H11N/c1-5(2)7-6(3)4/h7H,1,3H2,2,4H3	83.4	9	1	394.0	412.3	150.4	184.5	213.7	238.3	276.5	305.0	349.9
250	T	InChI=1S/C6H11N/c1-6(2)4-5-7-3/h4-5H,1-3H3/b7-5-	75.4	27	1	383.7	411.1	144.7	176.6	206.0	231.8	273.1	304.0	351.3
251	T	InChI=1S/C6H11NO2/c1-3-5-6(4-2)9-7-8/h3,6H,1,4-5H2,2H3/t6-/m0/s1	-71.1	3	2	459.5	462.9	178.9	218.6	252.7	280.5	322.3	352.1	397.3
252	T	InChI=1S/C6H13N/c1-5-6(2,3)7-4/h5,7H,1H2,2-4H3	7.7	27	2	396.3	418.0	163.4	201.3	234.5	262.2	305.1	337.1	387.9
253	T	InChI=1S/C6H13N/c1-5-7(4)6(2)3/h5-6H,1H2,2-4H3	6.2	27	2	393.8	415.4	155.5	194.2	228.3	257.1	302.5	336.4	389.7
254	T	InChI=1S/C6H13NO/c1-4-5-6(8)7(2)3/h4-5H2,1-3H3	-269.6	27	1	426.3	453.7	163.6	200.0	234.8	265.6	315.0	352.0	409.0
255	T	InChI=1S/C6H13NO/c1-4-7(5-2)6(3)8/h4-5H2,1-3H3	-284.3	27	1	421.0	448.4	167.1	206.2	241.8	272.2	320.1	355.6	410.5
256	T	InChI=1S/C6H15N/c1-3-5-7-6-4-2/h7H,3-6H2,1-2H3	-103.3	9	1	427.4	445.7	168.4	206.6	242.7	274.3	325.1	363.4	423.5
257	T	InChI=1S/C6H15N/c1-4-7(5-2)6-3/h4-6H2,1-3H3	-86.8	81	1	402.8	439.3	170.4	206.3	241.8	273.8	325.8	365.0	425.6
258	T	InChI=1S/C6H15N/c1-5(2)7-6(3)4/h5-7H,1-4H3	-127.0	81	1	407.4	443.9	168.7	210.7	248.5	280.6	330.6	367.6	424.9
259	T	InChI=1S/C6H6N/c1-3-5-7-6-4-2/h1-2H3	585.6	18	1	401.7	425.7	127.4	149.5	169.3	186.5	214.1	234.5	265.7
260	T	InChI=1S/C6H7N/c1-6(2)4-3-5-7/h6H,1-2H3	284.1	9	1	362.1	380.3	126.0	152.2	174.5	193.0	222.2	243.9	277.6
261	T	InChI=1S/C6H8N/c1-3-4-6(2)5-7/h3H,1,4H2,2H3	282.9	3	1	396.3	405.4	130.2	155.3	178.8	199.3	231.8	256.0	293.3
262	T	InChI=1S/C6H8N/c1-6(2)4-3-5-7/h3-4H,1-2H3	222.3	18	1	370.7	394.7	125.2	153.1	178.2	199.7	233.5	258.5	296.8
263	T	InChI=1S/C6H9N/c1-3-6(2)4-5-7/h4H,3H2,1-2H3/b6-4+	99.1	9	1	377.2	395.5	131.6	161.3	187.5	209.8	245.2	271.6	312.8
264	T	InChI=1S/C7H11N/c1-3-5-7(4-2)6-8/h3,7H,1,4-5H2,2H3/t7-/m1/s1	104.4	3	2	422.3	425.7	162.0	197.3	228.4	254.7	295.9	326.5	374.1
265	T	InChI=1S/C7H11N/c1-4-5-7(2,3)6-8/h4H,1,5H2,2-3H3	92.6	9	1	401.2	419.5	166.6	203.0	234.2	260.1	300.0	329.4	375.5
266	T	InChI=1S/C7H13N/c1-4-5-7(2,3)6-8/h4-5H2,1-3H3	-35.3	27	1	412.4	439.8	175.2	216.4	250.8	279.5	324.5	358.3	411.6
267	T	InChI=1S/C7H14N/c1-4-7(3)6-8-5-2/h6H,4-5H2,1-3H3	81.1	27	1	437.9	465.3	165.1	207.1	245.5	278.3	330.3	368.9	428.7
268	T	InChI=1S/C7H17N/c1-4-5-8-6-7(2)3/h7-8H,4-6H2,1-3H3	-130.0	27	2	466.2	487.9	194.1	239.9	281.8	317.7	374.8	417.6	484.1
269	T	InChI=1S/C8H19N/c1-3-5-7-9-8-6-4-2/h9H,3-8H2,1-2H3	-139.6	9	1	513.6	531.9	220.3	267.8	313.3	353.4	417.9	466.6	542.8
270	T	InChI=1S/CH2N/c1-2/h1-2H	274.4	1	1	228.4	228.4	38.2	43.0	47.5	51.5	57.8	62.8	70.9
271	T	InChI=1S/CH2N/c1-2/h1H2	239.3	1	1	224.0	224.0	37.6	42.3	46.9	51.0	57.9	63.2	71.6
272	T	InChI=1S/CH3N/c1-2/h2H,1H2	90.0	1	1	227.0	227.0	37.8	44.3	51.2	57.6	68.2	76.3	89.3
273	T	InChI=1S/CH3NO/c1-2-3/h1H3	68.6	3	1	260.3	269.4	52.1	60.4	68.5	75.8	87.5	96.3	110.0
274	T	InChI=1S/CH3NO2/c1-2(3)4/h1H3	-83.8	6	1	275.3	290.2	57.2	69.7	81.1	90.8	105.8	116.5	132.4
275	T	InChI=1S/CH3NO2/c1-4-2-3/h1H3	-69.6	3	1	286.5	295.7	64.3	74.9	84.9	93.7	107.6	117.8	133.2
276	T	InChI=1S/CH4N/c1-2/h1-2H2	153.7	2	1	246.0	251.7	51.0	60.1	67.9	74.5	84.9	93.1	107.0
277	T	InChI=1S/CH4N/c1-2/h2H,1H3	181.0	3	1	245.7	254.8	45.4	53.4	61.5	68.9	81.2	90.7	106.3
278	T	InChI=1S/CH4NO/c1-2-3/h2H,1H3	43.6	3	2	279.2	282.6	56.1	66.2	76.3	85.3	100.0	111.2	128.7
279	T	InChI=1S/CH4NO/c1-2-3/h3H,1H3	67.4	3	1	272.2	281.3	57.7	68.6	78.9	87.8	101.9	112.4	129.1
280	T	InChI=1S/CH5N/c1-2/h2H2,1H3	-19.5	3	1	241.5	250.6	49.5	59.4	69.2	78.0	92.8	104.6	124.1

281	T	InChI=1S/CH6N2/c1-3-2/h3H,2H2,1H3	97.0	3	2	278.6	282.0	72.8	88.1	101.2	112.2	129.8	143.4	165.9
282	V	InChI=1S/C3H8N2/c1-2-3(4)5/h2H,4-5H2,1H3	31.2	3	1	325.1	334.2	112.4	142.0	165.0	182.0	205.3	221.9	249.7
283	V	InChI=1S/C4H10N/c1-2-3-4-5/h5H,2-4H2,1H3	122.1	3	1	366.4	375.6	115.6	141.1	165.2	186.1	219.6	244.8	284.7
284	V	InChI=1S/C4H10N2/c1-2-3-6-4-5/h2,6H,1,3-5H2	88.2	1	2	384.9	379.2	136.4	165.4	190.8	212.0	244.7	269.1	308.1
285	V	InChI=1S/C4H10NO/c1-3-5(6)4-2/h3-4H2,1-2H3	-29.7	9	1	381.9	400.2	125.6	153.1	179.0	201.5	237.6	264.6	306.9
286	V	InChI=1S/C4H8N/c1-3-4(2)5/h5H,2-3H2,1H3	157.7	6	1	331.1	346.0	99.4	125.6	148.2	167.0	196.0	217.4	251.1
287	V	InChI=1S/C5H10N/c1-5(2)4-6-3/h4-5H,3H2,1-2H3	148.4	18	1	373.7	397.8	126.4	157.2	184.6	207.8	244.1	270.9	312.1
288	V	InChI=1S/C5H11N/c1-3-4-5(2)6/h4H,3,6H2,1-2H3/b5-4-	-21.5	9	1	373.1	391.3	128.4	161.8	191.3	216.2	254.9	283.4	327.8
289	V	InChI=1S/C5H11N/c1-3-5-6-4-2/h5H,3-4H2,1-2H3/b6-5-	-4.0	9	1	375.3	393.6	127.3	158.6	187.2	211.7	250.9	280.4	326.5
290	V	InChI=1S/C5H11NO2/c1-3-5(4-2)8-6-7/h5H,3-4H2,1-2H3	-180.1	9	1	420.8	439.1	167.6	203.5	234.9	260.9	300.5	329.3	373.9
291	V	InChI=1S/C5H12N2/c1-3-4-5(6)7-2/h3-5,7H,6H2,1-2H3/b4-3+/t5-/m1/s1	45.4	9	2	400.7	413.2	158.9	199.0	233.5	260.8	300.2	327.8	371.0
292	V	InChI=1S/C5H12N2/c1-3-4-5-7-6-2/h3-5H2,1-2H3	93.4	9	1	412.6	430.9	150.1	183.3	214.1	240.9	283.9	316.3	366.6
293	V	InChI=1S/C5H8N/c1-5(2)3-4-6/h3,5H,1-2H3	183.2	9	1	364.1	382.4	114.8	141.3	164.3	183.6	213.8	236.2	271.2
294	V	InChI=1S/C6H11N/c1-4-5-7-6(2)3/h5H,2,4H2,1,3H3/b7-5+	75.9	9	1	400.8	419.0	141.9	174.6	204.4	230.0	270.7	301.3	349.0
295	V	InChI=1S/C6H13N/c1-4-5-6(2,3)7/h4-5H,7H2,1-3H3/b5-4+	-33.3	27	1	402.3	429.7	159.4	197.0	230.0	257.8	301.3	333.9	386.0
296	V	InChI=1S/C6H13NO/c1-4-6(8)7(3)5-2/h4-5H2,1-3H3	-278.3	27	2	438.4	460.1	162.5	200.3	235.6	266.5	315.9	352.6	409.2
297	V	InChI=1S/C6H13NO2/c1-4-6(2,3)5-7(8)9/h4-5H2,1-3H3	-206.6	54	1	440.3	473.5	185.2	227.5	264.3	295.1	342.6	377.3	430.4
298	V	InChI=1S/C6H14N/c1-4-6(2,3)5-7/h5H,4,7H2,1-3H3	31.1	27	1	414.9	442.3	170.1	210.7	245.2	273.8	318.4	351.8	405.0
299	V	InChI=1S/C6H15N/c1-4-6(2,3)5-7/h4-5,7H2,1-3H3	-138.8	27	1	411.4	438.8	170.3	212.4	249.6	280.7	329.3	365.7	423.5
300	V	InChI=1S/C6H8N2/c7-5-3-1-2-4-6/h1-4H2	166.8	2	1	405.7	411.5	150.2	178.3	202.6	223.2	255.9	280.5	318.5

3. Differences between CBS-QB3 and GA approximated thermodynamic properties

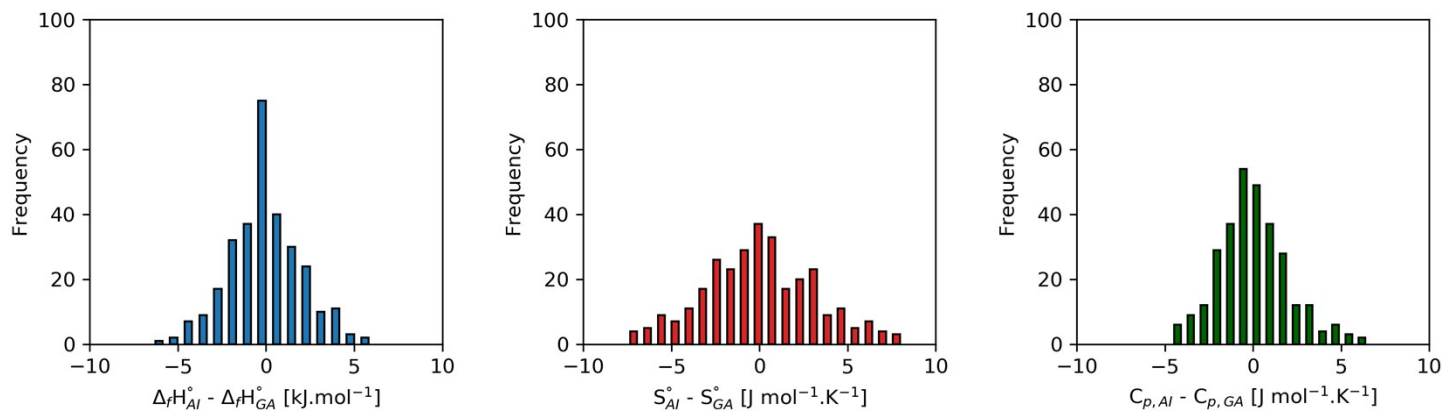


Figure S1: Distribution of the differences between *ab initio* calculated (AI) and group additive approximated values (GA) for the (a) standard enthalpy of formation [kJ mol⁻¹], (b) entropy and (c) heat capacity [J mol⁻¹ K⁻¹].

Table S3: Differences between the *ab initio* calculated (AI) and group additive approximated (GA) values for the standard enthalpy of formation [kJ mol⁻¹], intrinsic standard entropy [J mol⁻¹ K⁻¹] at 298 K and the heat capacities [J mol⁻¹ K⁻¹] at different temperatures for all 300 molecules. The GA approximations obtained with the final set of GAVs is used.

No.		InChI	$\Delta = AI - GA$									
			$\Delta_f H^{\circ}$	S_{int}°	C_p°							
					300 K	400 K	500 K	600 K	800 K	1000 K	1500 K	
1	T	InChI=1S/C2H2N/c1-2-3/h1,3H	1.0	-2.7	-1.4	-1.5	-1.7	-1.9	-2.2	-2.4	-2.7	
2	T	InChI=1S/C2H2N/c1-2-3/h1H2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
3	T	InChI=1S/C2H3N/c1-2-3/h1H,3H2	-3.1	0.5	-2.4	-2.2	-2.2	-2.3	-2.5	-2.7	-2.8	
4	T	InChI=1S/C2H3N/c1-2-3/h1H3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
5	T	InChI=1S/C2H3N/c1-2-3/h3H,1H2	-6.5	-2.7	1.9	2.3	2.3	2.1	1.6	1.2	0.7	
6	T	InChI=1S/C2H4N/c1-2-3/h1,3H2	-1.2	-2.1	4.7	4.4	3.8	3.2	2.3	1.9	1.3	
7	T	InChI=1S/C2H4N/c1-2-3/h1-2H,3H2	3.8	0.4	-0.7	-0.5	-0.2	0.1	0.5	0.6	0.4	
8	T	InChI=1S/C2H4N/c1-2-3/h2-3H,1H2	0.4	-3.9	1.7	1.8	1.6	1.3	0.8	0.5	0.2	
9	T	InChI=1S/C2H4N/c1-2-3/h2H,1H3	0.7	3.9	-1.5	-1.5	-1.4	-1.2	-0.8	-0.6	-0.3	

10	T	InChI=1S/C2H4N/c1-2-3/h3H,1H3	-0.4	-0.5	0.7	0.6	0.5	0.4	0.1	0.0	0.0
11	T	InChI=1S/C2H4N/c1-3-2/h1-2H2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
12	T	InChI=1S/C2H4N/c1-3-2/h1H,2H3	0.9	-2.0	-2.0	-1.2	-0.8	-0.6	-0.3	-0.3	-0.2
13	T	InChI=1S/C2H5N/c1-2-3/h2-3H,1H3/b3-2+	-0.2	2.2	-0.9	-0.7	-0.5	-0.5	-0.5	-0.5	-0.3
14	T	InChI=1S/C2H5N/c1-2-3/h2H,1,3H2	-2.8	4.1	-1.5	-1.7	-1.7	-1.6	-1.4	-1.1	-0.8
15	T	InChI=1S/C2H5N/c1-3-2/h1H2,2H3	0.2	2.4	0.2	0.5	0.6	0.6	0.6	0.5	0.2
16	T	InChI=1S/C2H5NO/c1-2(3)4/h1H3,3H2	-0.3	-1.9	0.2	1.0	1.5	1.6	1.1	0.6	0.0
17	T	InChI=1S/C2H5NO/c1-2-3-4/h2H2,1H3	-0.9	3.2	2.5	1.1	0.4	0.0	-0.1	-0.1	0.1
18	T	InChI=1S/C2H5NO/c1-3-2-4/h2H,1H3,3H1	4.2	-2.3	-0.3	0.0	0.2	0.3	0.4	0.4	0.3
19	T	InChI=1S/C2H5NO2/c1-2-5-3-4/h2H2,1H3	-0.1	8.2	3.1	1.9	1.2	0.7	0.3	0.2	0.1
20	T	InChI=1S/C2H6N/c1-2-3/h2H,3H2,1H3	-0.4	-0.9	0.6	0.3	0.4	0.6	0.9	1.0	0.9
21	T	InChI=1S/C2H6N/c1-2-3/h3H,2H2,1H3	-2.0	0.5	0.6	0.4	0.2	0.1	0.0	0.0	0.0
22	T	InChI=1S/C2H6N/c1-3-2/h1-2H3	-0.1	2.7	-1.5	-1.3	-1.1	-0.8	-0.4	-0.2	0.1
23	T	InChI=1S/C2H6N/c1-3-2/h3H,1H2,2H3	-0.4	-1.1	-0.4	-0.4	-0.5	-0.4	-0.2	0.0	0.3
24	T	InChI=1S/C2H6N2/c1-2(3)4/h1,3-4H2	-2.2	0.1	-0.2	0.1	0.3	0.4	0.2	0.1	0.0
25	T	InChI=1S/C2H6N2/c1-3-4-2/h1-2H3	-0.1	1.6	0.1	-0.1	-0.2	-0.2	-0.1	-0.1	-0.1
26	T	InChI=1S/C2H6NO/c1-2-3-4/h3H,2H2,1H3	1.1	-0.4	0.8	1.6	1.7	1.5	0.9	0.6	0.2
27	T	InChI=1S/C2H6NO/c1-2-3-4/h4H,2H2,1H3	0.1	0.2	-1.8	-1.4	-1.1	-0.8	-0.5	-0.3	-0.2
28	T	InChI=1S/C2H6NO/c1-3(2)4/h1-2H3	-0.5	0.9	0.1	-0.4	-0.4	-0.3	0.1	0.3	0.3
29	T	InChI=1S/C2H7N/c1-2-3/h2-3H2,1H3	-0.1	1.2	0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1
30	T	InChI=1S/C2H7N/c1-3-2/h3H,1-2H3	-1.7	1.0	-0.6	0.0	0.3	0.3	0.2	0.1	0.1
31	T	InChI=1S/C2H7NO/c1-2-3-4/h3-4H,2H2,1H3	-0.9	2.7	-3.7	-3.5	-2.9	-2.2	-1.3	-0.7	-0.3
32	T	InChI=1S/C2H7NO/c1-3(2)4/h4H,1-2H3	1.7	2.4	-1.0	-0.6	-0.4	-0.4	-0.6	-0.8	-0.6
33	T	InChI=1S/C2H8N2/c1-2(3)4/h2H,3-4H2,1H3	-0.6	0.8	-0.5	-0.2	-0.1	0.0	0.1	0.1	0.0
34	T	InChI=1S/C2H8N2/c1-2-4-3/h4H,2-3H2,1H3	0.5	-0.2	-1.1	-1.1	-1.2	-1.2	-1.0	-0.8	-0.3
35	T	InChI=1S/C2H8N2/c1-3-4-2/h3-4H,1-2H3	-0.8	2.1	-0.9	0.1	0.9	1.4	1.4	1.1	0.2
36	T	InChI=1S/C2H8N2/c1-4(2)3/h3H2,1-2H3	-0.8	1.0	-0.9	0.1	0.7	0.9	0.8	0.6	0.0
37	T	InChI=1S/C2H8N2/c1-4-2-3/h4H,2-3H2,1H3	-1.3	3.1	0.3	-0.2	-0.5	-0.7	-0.8	-0.7	-0.4
38	T	InChI=1S/C3H10N2/c1-2-3(4)5/h3H,2,4-5H2,1H3	0.2	-1.4	-0.9	-0.6	-0.2	0.0	0.3	0.3	0.2
39	T	InChI=1S/C3H10N2/c1-3(2)5-4/h3,5H,4H2,1-2H3	-0.6	-1.6	1.7	0.8	0.4	0.3	0.2	0.2	0.3
40	T	InChI=1S/C3H10N2/c1-3(4)5-2/h3,5H,4H2,1-2H3/t3-/m1/s1	0.4	0.6	1.4	0.8	0.3	-0.1	-0.3	-0.4	-0.2
41	T	InChI=1S/C3H10N2/c1-3-5(2)4/h3-4H2,1-2H3	0.0	1.1	0.0	0.0	0.2	0.4	0.6	0.5	0.2

42	T	InChI=1S/C3H10N2/c1-5(2)3-4/h3-4H2,1-2H3	1.3	-2.4	0.0	0.1	0.2	0.4	0.5	0.6	0.4
43	T	InChI=1S/C3H3N/c1-2-3-4/h1,3-4H/b4-3+	2.8	-5.6	-2.6	-2.4	-2.4	-2.4	-2.5	-2.6	-2.7
44	T	InChI=1S/C3H4N/c1-2-3-4/h2-3H,1H2	3.3	1.5	0.7	1.7	1.8	1.5	0.7	0.1	-0.3
45	T	InChI=1S/C3H4N/c1-2-3-4/h2H,1H3	-0.7	-0.4	1.9	1.2	0.9	0.8	0.7	0.7	0.6
46	T	InChI=1S/C3H4N/c1-2-3-4/h4H,1H3	0.5	6.3	0.5	0.6	0.7	0.9	1.1	1.2	1.4
47	T	InChI=1S/C3H4N/c1-3-4-2/h1H,2H3	0.7	-1.0	1.4	1.3	1.1	1.0	0.8	0.7	0.5
48	T	InChI=1S/C3H5N/c1-2-3-4/h2,4H,1H3	3.9	0.5	0.1	0.1	0.2	0.2	0.2	0.2	0.2
49	T	InChI=1S/C3H5N/c1-2-3-4/h2-4H,1H2/b4-3-	-1.2	-0.8	-0.6	0.8	1.6	1.9	1.9	1.6	1.0
50	T	InChI=1S/C3H5N/c1-2-3-4/h2H2,1H3	0.4	1.2	-1.1	-1.4	-1.3	-1.1	-0.7	-0.5	-0.2
51	T	InChI=1S/C3H5N/c1-2-3-4/h4H2,1H3	2.5	5.1	1.2	1.0	1.0	1.0	1.1	1.2	1.3
52	T	InChI=1S/C3H5N/c1-3-4-2/h1,4H,2H3	1.9	0.3	1.4	0.8	0.4	0.2	0.2	0.2	0.2
53	T	InChI=1S/C3H5N/c1-3-4-2/h1H2,2H3	1.7	-0.7	-0.6	-0.4	-0.4	-0.3	-0.3	-0.2	-0.2
54	T	InChI=1S/C3H5N/c1-3-4-2/h3H,1-2H2	0.8	5.8	2.0	1.2	0.4	-0.1	-0.3	-0.3	-0.1
55	T	InChI=1S/C3H6N/c1-2-3-4/h2,4H,1,3H2	2.8	2.1	-2.8	-2.7	-2.4	-1.9	-1.1	-0.6	-0.1
56	T	InChI=1S/C3H6N/c1-2-3-4/h2-3H,1,4H2	1.9	-4.8	3.0	3.0	2.6	2.2	1.4	0.8	0.0
57	T	InChI=1S/C3H6N/c1-2-3-4/h2-4H,1H3	-2.8	-0.9	-0.9	-1.0	-0.9	-0.8	-0.6	-0.4	-0.2
58	T	InChI=1S/C3H6N/c1-2-3-4/h3-4H,1-2H2/b4-3+	0.2	-2.7	4.0	3.0	2.4	2.0	1.4	1.1	0.7
59	T	InChI=1S/C3H6N/c1-2-3-4/h4H,2H2,1H3	-0.4	2.8	-0.2	-0.3	-0.3	-0.3	-0.2	-0.1	0.0
60	T	InChI=1S/C3H6N/c1-3(2)4/h1-2H3	1.2	0.8	0.4	-0.1	-0.3	-0.3	-0.2	-0.1	-0.1
61	T	InChI=1S/C3H6N/c1-3(2)4/h4H,1H2,2H3	0.8	7.3	-0.2	-0.3	-0.2	-0.1	0.2	0.4	0.3
62	T	InChI=1S/C3H6N/c1-3-4-2/h1,3-4H,2H3	4.1	4.5	3.0	2.3	1.8	1.4	0.8	0.4	-0.3
63	T	InChI=1S/C3H6N/c1-3-4-2/h2H,3H2,1H3	1.5	6.4	-0.2	-1.0	-1.3	-1.3	-1.1	-1.0	-0.6
64	T	InChI=1S/C3H6N/c1-3-4-2/h3-4H,1-2H2	-3.6	2.9	-0.7	-0.8	-0.9	-1.0	-1.1	-1.1	-0.8
65	T	InChI=1S/C3H6N/c1-3-4-2/h3H,1H2,2H3	2.5	-1.6	1.0	1.1	0.9	0.7	0.2	-0.1	-0.4
66	T	InChI=1S/C3H6N/c1-3-4-2/h3H,2H2,1H3	-1.0	-7.3	1.2	0.8	0.6	0.4	0.1	0.0	0.3
67	T	InChI=1S/C3H6N/c1-3-4-2/h4H,1H2,2H3	1.6	3.0	-2.9	-4.0	-4.6	-4.8	-4.3	-3.4	-1.9
68	T	InChI=1S/C3H7N/c1-2-3-4/h2-3H,4H2,1H3/b3-2+	4.6	2.9	0.1	-0.2	-0.2	-0.2	-0.4	-0.6	-0.9
69	T	InChI=1S/C3H7N/c1-2-3-4/h2H,1,3-4H2	1.1	-2.2	0.7	1.5	1.5	1.3	0.9	0.6	0.3
70	T	InChI=1S/C3H7N/c1-2-3-4/h3-4H,2H2,1H3/b4-3+	-0.2	3.7	-2.9	-1.9	-1.2	-0.8	-0.4	-0.2	0.0
71	T	InChI=1S/C3H7N/c1-3(2)4/h1,4H2,2H3	-2.6	0.2	-0.8	-0.9	-0.8	-0.5	-0.1	0.2	0.4
72	T	InChI=1S/C3H7N/c1-3(2)4/h4H,1-2H3	-1.2	-0.8	-0.4	0.1	0.3	0.3	0.2	0.1	0.1
73	T	InChI=1S/C3H7N/c1-3-4-2/h2-3H2,1H3	1.3	-1.5	1.3	1.1	0.8	0.6	0.4	0.3	0.0

74	T	InChI=1S/C3H7N/c1-3-4-2/h3-4H,1H2,2H3	-1.8	-2.6	-1.1	-1.2	-1.6	-1.9	-2.2	-2.1	-0.9
75	T	InChI=1S/C3H7N/c1-3-4-2/h3H,1-2H3/b4-3-	0.2	-1.3	0.4	0.5	0.5	0.3	0.1	-0.1	-0.2
76	T	InChI=1S/C3H7NO/c1-2-3(4)5/h2H2,1H3,4H2	-1.2	6.9	-1.4	-3.6	-5.0	-5.3	-4.7	-3.7	-1.8
77	T	InChI=1S/C3H7NO/c1-2-3-4-5/h2-3H2,1H3	0.0	0.4	-2.3	-1.0	-0.4	-0.2	-0.1	0.0	0.1
78	T	InChI=1S/C3H7NO/c1-3(2)4-5/h3H,1-2H3	-0.2	-1.5	-3.5	-3.1	-2.6	-2.1	-1.3	-0.9	-0.3
79	T	InChI=1S/C3H7NO/c1-3(5)4-2/h1-2H3,4H1	-1.7	-1.7	1.4	0.5	-0.1	-0.4	-0.6	-0.6	-0.5
80	T	InChI=1S/C3H7NO/c1-4(2)3-5/h3H,1-2H3	-4.2	2.3	0.3	0.0	-0.2	-0.3	-0.4	-0.4	-0.3
81	T	InChI=1S/C3H7NO2/c1-2-3-4(5)6/h2-3H2,1H3	-0.4	-0.2	-3.9	-2.3	-1.4	-0.8	-0.2	0.1	0.6
82	T	InChI=1S/C3H7NO2/c1-2-3-6-4-5/h2-3H2,1H3	-0.1	-4.1	-2.8	-1.5	-0.9	-0.6	-0.4	-0.3	-0.1
83	T	InChI=1S/C3H7NO2/c1-3(2)4(5)6/h3H,1-2H3	2.6	5.7	-2.5	-2.4	-2.3	-2.1	-1.7	-1.2	-0.5
84	T	InChI=1S/C3H7NO2/c1-3(2)6-4-5/h3H,1-2H3	2.2	4.3	-2.6	-3.5	-4.3	-4.7	-4.6	-4.1	-3.0
85	T	InChI=1S/C3H8N/c1-2-3-4/h1-4H2	-3.3	-0.7	-1.8	-0.8	-0.2	0.1	0.2	0.1	0.1
86	T	InChI=1S/C3H8N/c1-2-3-4/h2H,3-4H2,1H3	-0.2	-2.6	1.7	1.7	1.5	1.3	0.9	0.6	0.3
87	T	InChI=1S/C3H8N/c1-2-3-4/h3H,2,4H2,1H3	1.0	-1.5	-3.2	-2.0	-1.2	-0.7	-0.4	-0.2	-0.1
88	T	InChI=1S/C3H8N/c1-2-3-4/h4H,2-3H2,1H3	2.0	1.0	-1.8	-0.9	-0.5	-0.3	-0.2	-0.2	-0.1
89	T	InChI=1S/C3H8N/c1-3(2)4/h3-4H,1-2H3	-0.1	3.4	0.1	0.0	-0.3	-0.5	-0.7	-0.6	-0.4
90	T	InChI=1S/C3H8N/c1-3(2)4/h4H2,1-2H3	-3.6	-0.1	3.5	2.3	1.4	0.8	0.3	0.1	0.0
91	T	InChI=1S/C3H8N/c1-3-4-2/h3H2,1-2H3	0.0	-4.5	0.3	0.1	0.0	-0.1	-0.1	-0.1	-0.1
92	T	InChI=1S/C3H8N/c1-3-4-2/h4H,1,3H2,2H3	-1.7	-4.7	4.6	3.4	2.5	1.9	1.2	0.9	0.6
93	T	InChI=1S/C3H8N/c1-3-4-2/h4H,2-3H2,1H3	1.2	4.0	-1.4	-1.3	-1.3	-1.3	-1.1	-1.0	-0.7
94	T	InChI=1S/C3H8N2/c1-2-3(4)5/h2-3H,1,4-5H2	3.4	5.2	-1.2	-4.6	-6.8	-7.5	-6.7	-5.0	-2.4
95	T	InChI=1S/C3H8N2/c1-3(4)5-2/h5H,1,4H2,2H3	-0.5	-0.8	-2.0	-1.8	-0.8	0.5	1.9	2.1	1.0
96	T	InChI=1S/C3H8N2/c1-3-5-4-2/h3H2,1-2H3	0.1	-0.7	0.6	0.0	-0.2	-0.3	-0.2	-0.2	-0.1
97	T	InChI=1S/C3H8NO/c1-3(2)4-5/h3,5H,1-2H3	1.3	1.2	0.8	0.6	0.3	0.0	-0.3	-0.4	-0.4
98	T	InChI=1S/C3H8NO/c1-3(2)4-5/h3-4H,1-2H3	0.2	0.3	1.4	1.2	0.7	0.2	-0.3	-0.5	-0.4
99	T	InChI=1S/C3H8NO/c1-3-4(2)5/h3H2,1-2H3	-1.1	1.8	-1.9	-2.2	-2.0	-1.6	-1.0	-0.6	-0.2
100	T	InChI=1S/C3H9N/c1-2-3-4/h2-4H2,1H3	0.7	2.1	-1.6	-1.1	-0.7	-0.5	-0.4	-0.4	-0.3
101	T	InChI=1S/C3H9N/c1-3(2)4/h3H,4H2,1-2H3	-3.4	2.6	-0.5	-0.3	-0.2	-0.2	-0.2	-0.2	0.0
102	T	InChI=1S/C3H9N/c1-3-4-2/h4H,3H2,1-2H3	-1.4	-0.2	0.6	0.3	0.1	-0.1	-0.2	-0.2	0.0
103	T	InChI=1S/C3H9N/c1-4(2)3/h1-3H3	-0.2	0.4	1.1	0.4	0.1	0.0	-0.1	-0.1	-0.1
104	T	InChI=1S/C3H9NO/c1-3(2)4-5/h3-5H,1-2H3	-2.2	1.6	-2.0	-2.7	-2.5	-1.9	-1.0	-0.5	-0.1
105	T	InChI=1S/C3H9NO/c1-3-4(2)5/h5H,3H2,1-2H3	0.9	-1.0	1.8	2.0	1.7	1.4	0.8	0.4	0.1

106	T	InChI=1S/C4H10N/c1-2-3-4-5/h2H,3-5H2,1H3	-1.7	-2.4	-2.4	-0.9	0.0	0.4	0.6	0.4	0.2
107	T	InChI=1S/C4H10N/c1-2-3-4-5/h3H,2,4-5H2,1H3	1.6	0.8	-4.5	-2.1	-1.0	-0.6	-0.5	-0.6	-0.6
108	T	InChI=1S/C4H10N/c1-2-3-4-5/h4H,2-3,5H2,1H3	1.4	-2.8	-3.8	-1.9	-0.7	-0.1	0.4	0.6	0.5
109	T	InChI=1S/C4H10N/c1-3-4(2)5/h3,5H2,1-2H3	-4.4	0.1	-0.9	-0.1	0.3	0.6	0.7	0.7	0.5
110	T	InChI=1S/C4H10N/c1-3-5-4-2/h3,5H,4H2,1-2H3	-3.0	4.4	4.2	0.9	-0.6	-1.2	-1.5	-1.4	-0.9
111	T	InChI=1S/C4H10N/c1-3-5-4-2/h3-4H2,1-2H3	0.1	1.8	1.2	1.3	1.1	0.9	0.5	0.3	0.0
112	T	InChI=1S/C4H10N/c1-3-5-4-2/h5H,1,3-4H2,2H3	-1.7	-3.5	5.4	3.1	1.7	1.0	0.5	0.4	0.4
113	T	InChI=1S/C4H10N/c1-4(2)3-5/h4-5H,3H2,1-2H3	-2.6	-4.1	2.0	1.5	1.4	1.2	0.9	0.6	0.0
114	T	InChI=1S/C4H10N2/c1-3-4(5)6-2/h3-4,6H,1,5H2,2H3/t4-/m1/s1	-1.3	-3.1	1.6	3.9	4.7	4.5	3.3	2.2	0.9
115	T	InChI=1S/C4H10N2/c1-3-5-6-4-2/h3-4H2,1-2H3	0.0	0.5	1.1	0.2	-0.2	-0.3	-0.3	-0.2	0.0
116	T	InChI=1S/C4H11N/c1-2-3-4-5/h2-5H2,1H3	1.6	-0.6	-2.3	-1.7	-1.3	-1.0	-0.7	-0.5	-0.3
117	T	InChI=1S/C4H11N/c1-3-4(2)5/h4H,3,5H2,1-2H3/t4-/m1/s1	0.4	0.1	0.1	0.2	0.2	0.2	0.1	0.0	0.0
118	T	InChI=1S/C4H11N/c1-3-5-4-2/h5H,3-4H2,1-2H3	2.4	-0.7	2.0	0.9	0.2	-0.2	-0.4	-0.3	-0.1
119	T	InChI=1S/C4H11N/c1-4(2)3-5/h4H,3,5H2,1-2H3	1.3	-0.6	-0.7	-1.3	-1.1	-0.9	-0.5	-0.4	-0.4
120	T	InChI=1S/C4H11N/c1-4(2)5-3/h4-5H,1-3H3	-1.3	0.7	-0.5	-0.6	-0.7	-0.7	-0.7	-0.5	-0.2
121	T	InChI=1S/C4H11N/c1-4(2,3)5/h5H2,1-3H3	-3.7	2.1	2.1	1.7	1.4	1.2	0.9	0.7	0.4
122	T	InChI=1S/C4H11N/c1-4-5(2)3/h4H2,1-3H3	-1.7	3.0	-1.6	-0.7	-0.5	-0.5	-0.6	-0.6	-0.5
123	T	InChI=1S/C4H11NO/c1-3-5(6)4-2/h6H,3-4H2,1-2H3	0.5	-5.8	4.9	4.8	3.9	3.2	2.2	1.6	1.0
124	T	InChI=1S/C4H12N2/c1-4-6(3)5-2/h5H,4H2,1-3H3	0.8	-2.1	0.9	-0.1	-0.9	-1.4	-1.4	-1.1	-0.2
125	T	InChI=1S/C4H3N/c1-2-3-4-5/h1H3	0.9	0.0	-0.2	-0.1	0.0	0.1	0.2	0.2	0.1
126	T	InChI=1S/C4H4N/c1-2-3-4-5/h2-3H,1H2	4.4	-3.3	2.7	3.0	2.7	2.2	1.5	1.1	0.5
127	T	InChI=1S/C4H4N/c1-3-5-4-2/h1,4H,2H2	-0.1	-7.5	-4.7	-4.2	-3.9	-3.9	-3.9	-3.9	-3.9
128	T	InChI=1S/C4H5N/c1-2-3-4-5/h2-3H,1H3/b3-2+	5.7	-0.8	1.9	2.0	1.8	1.4	1.0	0.7	0.4
129	T	InChI=1S/C4H5N/c1-2-3-4-5/h2H,1,3H2	2.4	-0.3	0.8	0.9	0.8	0.6	0.4	0.3	0.2
130	T	InChI=1S/C4H5N/c1-2-3-4-5/h4-5H,1H3/b5-4+	-2.2	0.4	2.3	1.9	1.7	1.6	1.5	1.5	1.5
131	T	InChI=1S/C4H5N/c1-3-5-4-2/h1,4-5H,2H2	-1.0	2.1	1.0	0.7	0.5	0.3	0.0	-0.1	-0.2
132	T	InChI=1S/C4H5N/c1-4(2)3-5/h1H2,2H3	2.2	1.4	-0.4	-0.4	-0.3	-0.3	-0.2	-0.2	-0.1
133	T	InChI=1S/C4H6N/c1-2-3-4-5/h3H,2H2,1H3	-0.3	0.6	-1.7	-0.8	-0.3	-0.1	0.0	0.0	0.1
134	T	InChI=1S/C4H6N/c1-3-4-5-2/h3H,2H2,1H3	1.3	-1.2	0.9	1.0	0.9	0.7	0.4	0.1	-0.3
135	T	InChI=1S/C4H6N/c1-3-5-4-2/h1H,4H2,2H3	-0.1	0.9	-2.4	-1.7	-1.2	-0.9	-0.5	-0.4	-0.2
136	T	InChI=1S/C4H6N/c1-3-5-4-2/h3-4H,1-2H2	-4.2	-1.3	-3.6	-2.5	-0.7	0.6	1.7	1.8	1.4
137	T	InChI=1S/C4H6N/c1-3-5-4-2/h4H,1H2,2H3	-4.1	-1.6	1.3	1.1	0.9	0.7	0.6	0.5	0.5

138	T	InChI=1S/C4H6N/c1-4(2)3-5/h1-2H3	-0.2	2.5	-0.8	-0.7	-0.6	-0.4	-0.1	0.0	0.2
139	T	InChI=1S/C4H7N/c1-2-3-4-5/h2,5H2,1H3	0.7	-5.7	1.1	1.2	1.2	1.3	1.4	1.4	1.4
140	T	InChI=1S/C4H7N/c1-2-3-4-5/h2-3H2,1H3	-2.5	-0.5	-2.6	-1.8	-1.1	-0.6	-0.3	-0.2	-0.2
141	T	InChI=1S/C4H7N/c1-2-3-4-5/h2-5H,1H3/b3-2+,5-4-	4.0	0.3	0.0	-0.2	-0.6	-1.0	-1.1	-1.0	-0.7
142	T	InChI=1S/C4H7N/c1-3-4-5-2/h3-4H,1H2,2H3/b5-4-	-2.3	-4.0	1.1	2.2	2.6	2.7	2.4	2.0	1.2
143	T	InChI=1S/C4H7N/c1-3-4-5-2/h3-4H,2H2,1H3/b4-3+	-0.4	-5.1	-3.3	-1.7	-0.1	0.9	1.6	1.4	0.8
144	T	InChI=1S/C4H7N/c1-3-5-4-2/h1,4H2,2H3	0.9	3.0	-1.4	-2.0	-2.1	-2.0	-1.6	-1.2	-0.7
145	T	InChI=1S/C4H7N/c1-3-5-4-2/h1,5H,4H2,2H3	0.6	4.4	-1.4	-0.9	-0.6	-0.4	-0.2	-0.2	-0.2
146	T	InChI=1S/C4H7N/c1-3-5-4-2/h3-4H,1H2,2H3/b5-4-	-0.4	-0.7	1.2	0.5	-0.3	-0.9	-1.2	-1.2	-0.7
147	T	InChI=1S/C4H7N/c1-3-5-4-2/h3-5H,1-2H2	-4.7	1.7	3.1	3.1	2.6	2.3	2.2	2.3	2.3
148	T	InChI=1S/C4H7N/c1-4(2)3-5/h4H,1-2H3	2.0	4.3	-1.4	-1.3	-1.2	-1.0	-0.8	-0.6	-0.2
149	T	InChI=1S/C4H7N/c1-4(2)5-3/h1,3H2,2H3	1.9	-0.6	-1.5	-0.8	-0.3	-0.1	0.2	0.3	0.2
150	T	InChI=1S/C4H8N/c1-3-4(2)5/h3H,1,5H2,2H3	-2.2	-2.5	2.4	2.6	2.5	2.4	2.0	1.8	1.2
151	T	InChI=1S/C4H8N/c1-3-4-5-2/h3-5H,1H2,2H3	-4.2	1.4	-1.6	-1.9	-2.1	-2.1	-1.8	-1.3	-0.1
152	T	InChI=1S/C4H8N/c1-3-4-5-2/h4H,2-3H2,1H3	-0.6	5.0	-1.4	-0.6	-0.3	0.0	0.2	0.3	0.2
153	T	InChI=1S/C4H8N/c1-3-5-4-2/h5H,1,4H2,2H3	1.3	-4.2	-1.7	-0.1	0.6	0.7	0.3	-0.1	-0.4
154	T	InChI=1S/C4H8N/c1-4(2)3-5/h3,5H,1-2H3	1.2	3.4	0.9	0.5	0.2	0.0	-0.1	-0.1	0.0
155	T	InChI=1S/C4H8N/c1-4(2)3-5/h3H,1,5H2,2H3	2.3	3.4	-1.3	-1.1	-0.6	-0.1	0.4	0.5	0.1
156	T	InChI=1S/C4H8N/c1-4(2)3-5/h4-5H,1-2H3	0.8	-2.3	-0.6	-0.3	-0.2	-0.1	0.0	0.1	0.1
157	T	InChI=1S/C4H8N/c1-4(2)5-3/h1H2,2-3H3	-1.6	-0.5	-1.8	-1.6	-1.5	-1.4	-1.2	-1.0	-0.7
158	T	InChI=1S/C4H8N/c1-4(2)5-3/h3H2,1-2H3	-1.6	6.1	0.5	0.0	-0.8	-1.6	-2.4	-2.5	-1.3
159	T	InChI=1S/C4H8N/c1-4-5(2)3/h1H2,2-3H3	-1.7	3.3	-0.2	-0.3	0.2	0.9	1.7	1.7	0.9
160	T	InChI=1S/C4H9N/c1-2-3-4-5/h2-3H,4-5H2,1H3/b3-2+	0.1	4.8	-0.8	-0.7	-0.7	-0.7	-0.6	-0.5	-0.3
161	T	InChI=1S/C4H9N/c1-2-3-4-5/h3-4H,2,5H2,1H3/b4-3+	3.3	-1.6	1.2	1.2	1.3	1.3	1.1	0.8	0.1
162	T	InChI=1S/C4H9N/c1-3-4(2)5/h2-3,5H2,1H3	-1.9	-2.5	-1.1	-0.9	-0.4	0.1	0.7	0.9	0.7
163	T	InChI=1S/C4H9N/c1-3-4(2)5/h3-4H,1,5H2,2H3/t4-/m0/s1	-0.6	-2.2	2.6	2.6	2.1	1.6	0.9	0.5	0.3
164	T	InChI=1S/C4H9N/c1-3-4-5-2/h3,5H,1,4H2,2H3	-0.3	-3.3	-1.0	0.2	0.7	0.8	0.7	0.5	0.3
165	T	InChI=1S/C4H9N/c1-3-4-5-2/h4H,3H2,1-2H3/b5-4-	0.0	-0.8	-1.0	-0.8	-0.7	-0.6	-0.4	-0.3	-0.1
166	T	InChI=1S/C4H9N/c1-3-5-4-2/h3,5H,1,4H2,2H3	-0.4	4.3	0.2	-0.7	-1.0	-1.0	-0.6	-0.1	0.4
167	T	InChI=1S/C4H9N/c1-3-5-4-2/h3H,4H2,1-2H3/b5-3-	0.2	-0.6	0.6	0.8	0.7	0.4	0.0	-0.2	-0.3
168	T	InChI=1S/C4H9N/c1-4(2)3-5/h1,3,5H2,2H3	-1.1	5.8	0.1	-2.7	-3.3	-3.1	-2.2	-1.5	-0.7
169	T	InChI=1S/C4H9N/c1-4(2)3-5/h3-5H,1-2H3/b5-3+	0.4	2.5	-1.5	-1.4	-1.2	-1.1	-0.8	-0.6	-0.3

170	T	InChI=1S/C4H9N/c1-4(2)3-5/h3H,5H2,1-2H3	-2.1	2.4	-0.5	-0.7	-1.0	-1.1	-1.0	-0.8	-0.3
171	T	InChI=1S/C4H9N/c1-4(2)5-3/h1-3H3	1.9	-0.2	-0.8	-0.1	0.0	-0.1	-0.4	-0.6	-0.6
172	T	InChI=1S/C4H9N/c1-4(2)5-3/h5H,1H2,2-3H3	-2.8	-2.9	1.9	2.5	2.4	2.2	1.8	1.5	0.9
173	T	InChI=1S/C4H9N/c1-4-5(2)3/h4H,1H2,2-3H3	-2.0	7.9	-0.8	-1.2	-1.4	-1.2	-0.7	-0.2	0.1
174	T	InChI=1S/C4H9NO/c1-2-3-4(5)6/h2-3H2,1H3,5H2	-1.5	2.3	-1.9	-2.5	-3.1	-3.3	-2.9	-2.3	-1.0
175	T	InChI=1S/C4H9NO/c1-3(2)4(5)6/h3H,1-2H3,5H2	0.7	-4.1	3.2	3.5	3.7	3.6	2.9	2.1	1.0
176	T	InChI=1S/C4H9NO/c1-3-4(2)5-6/h4H,3H2,1-2H3/t4-/m1/s1	0.2	4.5	-1.0	-1.1	-0.8	-0.6	-0.3	-0.2	-0.1
177	T	InChI=1S/C4H9NO/c1-3-5-4(2)6/h3H2,1-2H3,5H1	-2.4	4.0	-1.2	-0.5	-0.1	0.1	0.2	0.2	0.2
178	T	InChI=1S/C4H9NO/c1-4(2)3-5-6/h4H,3H2,1-2H3	0.9	-3.7	-0.2	-0.1	0.0	0.1	0.2	0.1	-0.1
179	T	InChI=1S/C4H9NO/c1-4(6)5(2)3/h1-3H3	1.0	6.8	-0.3	-1.8	-2.5	-2.7	-2.6	-2.3	-1.7
180	T	InChI=1S/C4H9NO2/c1-2-3-4-5(6)7/h2-4H2,1H3	-0.4	-2.4	-3.5	-2.1	-1.2	-0.8	-0.3	0.0	0.5
181	T	InChI=1S/C4H9NO2/c1-3-4(2)5(6)7/h4H,3H2,1-2H3/t4-/m1/s1	0.1	0.5	0.4	0.2	0.0	-0.2	-0.3	-0.3	-0.2
182	T	InChI=1S/C4H9NO2/c1-3-4(2)7-5-6/h4H,3H2,1-2H3/t4-/m1/s1	0.7	1.5	-2.0	-2.3	-2.7	-2.9	-2.9	-2.8	-2.4
183	T	InChI=1S/C4H9NO2/c1-4(2)3-5(6)7/h4H,3H2,1-2H3	-1.0	-0.2	-0.9	-1.2	-1.0	-0.8	-0.4	-0.3	-0.1
184	T	InChI=1S/C4H9NO2/c1-4(2)3-7-5-6/h4H,3H2,1-2H3	0.2	-4.1	-0.2	-0.4	-0.2	-0.1	0.1	0.1	0.0
185	T	InChI=1S/C5H10N/c1-3-4-5(2)6/h3-4H,6H2,1-2H3	0.3	-1.3	0.1	0.2	0.5	0.7	1.0	1.0	0.7
186	T	InChI=1S/C5H10N/c1-3-5(2)4-6/h4,6H,3H2,1-2H3	-0.9	-0.3	0.6	1.7	2.1	2.1	1.8	1.5	0.9
187	T	InChI=1S/C5H10N/c1-4-5(2)6-3/h4,6H,1H2,2-3H3	1.9	3.8	-2.6	-2.8	-3.0	-3.1	-3.0	-2.7	-1.9
188	T	InChI=1S/C5H10N/c1-4-6-5(2)3/h2,4H2,1,3H3	-0.8	2.2	0.8	0.5	0.6	0.7	1.0	1.1	1.1
189	T	InChI=1S/C5H10N/c1-4-6-5(2)3/h4H,1-3H3	1.6	-6.1	-0.5	0.0	0.8	1.6	2.4	2.5	1.3
190	T	InChI=1S/C5H10N/c1-5(2)4-6-3/h4H,1-3H3	-0.5	0.5	1.0	-0.3	-0.7	-0.7	-0.6	-0.4	-0.1
191	T	InChI=1S/C5H11N/c1-2-3-4-5-6/h3-4H,2,5-6H2,1H3/b4-3+	-0.5	-0.4	3.0	2.8	2.2	1.7	1.0	0.6	0.3
192	T	InChI=1S/C5H11N/c1-3-4-5-6-2/h3-4,6H,5H2,1-2H3/b4-3+	-1.5	-3.3	0.3	0.8	0.9	0.9	0.6	0.4	0.2
193	T	InChI=1S/C5H11N/c1-3-5(2)4-6/h4-6H,3H2,1-2H3	-4.1	0.5	2.9	2.8	2.5	2.2	1.5	1.1	0.6
194	T	InChI=1S/C5H11N/c1-3-5(2)4-6/h4H,3,6H2,1-2H3/b5-4-	-2.2	-2.0	0.1	-0.2	-0.4	-0.4	-0.3	-0.1	0.1
195	T	InChI=1S/C5H11N/c1-3-5-6-4-2/h3,6H,1,4-5H2,2H3	-0.4	-2.7	0.7	0.8	0.7	0.6	0.4	0.3	0.2
196	T	InChI=1S/C5H11N/c1-4(2)5(3)6/h5H,1,6H2,2-3H3/t5-/m1/s1	-1.1	3.3	-1.7	-1.6	-1.3	-1.0	-0.6	-0.5	-0.4
197	T	InChI=1S/C5H11N/c1-4-5(2)6-3/h4-6H,1H2,2-3H3/t5-/m0/s1	1.7	-1.1	-0.9	-0.9	-0.8	-0.6	-0.3	-0.1	0.1
198	T	InChI=1S/C5H11N/c1-4-5(2)6-3/h4H2,1-3H3/b6-5+	-0.2	-1.9	0.6	0.3	0.1	0.0	-0.1	-0.2	-0.2
199	T	InChI=1S/C5H11N/c1-4-5(2,3)6/h4H,1,6H2,2-3H3	-1.4	0.4	-0.5	-0.5	-0.5	-0.4	-0.3	-0.2	0.0
200	T	InChI=1S/C5H11N/c1-4-6(3)5-2/h4H,1,5H2,2-3H3	0.1	-4.9	0.8	0.6	0.2	-0.2	-0.7	-0.9	-0.5
201	T	InChI=1S/C5H11N/c1-4-6-5(2)3/h4H2,1-3H3	-1.7	2.2	0.1	-0.2	-0.1	0.1	0.5	0.8	0.9

202	T	InChI=1S/C5H11N/c1-4-6-5(2)3/h6H,2,4H2,1,3H3	-2.1	-3.8	3.0	3.0	2.7	2.4	2.1	2.0	1.7
203	T	InChI=1S/C5H11N/c1-5(2)4-6-3/h4,6H,1-3H3	4.3	-0.4	0.4	1.0	1.4	1.5	1.3	0.9	0.2
204	T	InChI=1S/C5H11NO/c1-3-5(4-2)6-7/h5H,3-4H2,1-2H3	0.0	-3.0	4.5	4.2	3.4	2.7	1.7	1.1	0.4
205	T	InChI=1S/C5H11NO/c1-4-5(7)6(2)3/h4H2,1-3H3	1.9	-0.7	0.2	-0.8	-1.3	-1.4	-1.0	-0.7	-0.1
206	T	InChI=1S/C5H11NO/c1-5(2,3)4(6)7/h1-3H3,6H2	2.3	-3.2	-0.1	1.6	2.9	3.5	3.6	3.2	1.9
207	T	InChI=1S/C5H11NO2/c1-3-5(4-2)6(7)8/h5H,3-4H2,1-2H3	-2.7	-6.2	2.1	2.3	2.4	2.3	2.0	1.5	0.7
208	T	InChI=1S/C5H11NO2/c1-5(2,3)4-6(7)8/h4H2,1-3H3	-1.0	5.8	1.8	0.3	-0.3	-0.5	-0.6	-0.5	-0.5
209	T	InChI=1S/C5H12N/c1-4-5(2)6-3/h6H,4H2,1-3H3	4.4	-1.7	-0.7	-0.7	-0.3	0.1	0.4	0.5	0.5
210	T	InChI=1S/C5H12N2/c1-3-5-7-6-4-2/h3-5H2,1-2H3	-0.1	1.1	-1.0	-0.4	0.0	0.1	0.2	0.1	0.0
211	T	InChI=1S/C5H13N/c1-2-3-4-5-6/h2-6H2,1H3	2.3	-3.0	-2.0	-1.8	-1.4	-1.1	-0.8	-0.6	-0.3
212	T	InChI=1S/C5H13N/c1-3-4-5(2)6/h5H,3-4,6H2,1-2H3/t5-/m1/s1	-1.0	-2.4	-0.3	0.5	0.6	0.5	0.3	0.2	0.2
213	T	InChI=1S/C5H13N/c1-3-5(6)4-2/h5H,3-4,6H2,1-2H3	1.9	-2.6	1.5	0.8	0.5	0.3	0.1	0.0	0.0
214	T	InChI=1S/C5H13N/c1-4-5(2,3)6/h4,6H2,1-3H3	0.3	-0.4	-0.5	-0.3	-0.1	0.1	0.3	0.3	0.2
215	T	InChI=1S/C5H13N/c1-4-6-5(2)3/h5-6H,4H2,1-3H3	-1.0	1.3	-0.6	-0.3	-0.3	-0.4	-0.2	0.0	0.3
216	T	InChI=1S/C5H13N/c1-5(2,3)6-4/h6H,1-4H3	3.4	-1.6	-1.6	-1.4	-1.4	-1.3	-1.2	-1.0	-0.6
217	T	InChI=1S/C5H4N/c1-3-5-6-4-2/h2H,1H3	0.3	-5.9	-1.8	-1.6	-1.6	-1.7	-1.8	-1.9	-2.1
218	T	InChI=1S/C5H6N/c1-2-3-4-5-6/h2-4H,1H3	-0.9	-0.1	1.4	1.4	1.2	1.0	0.6	0.5	0.3
219	T	InChI=1S/C5H6N/c1-3-5(2)4-6/h3H,2H2,1H3	3.4	-1.2	0.8	1.0	0.9	0.8	0.7	0.5	0.4
220	T	InChI=1S/C5H6N/c1-3-5-6-4-2/h4H,2H2,1H3	1.1	-0.3	-1.1	-0.9	-0.7	-0.4	-0.1	0.0	0.1
221	T	InChI=1S/C5H6N/c1-4-6-5(2)3/h1H,2H2,3H3	-1.1	7.9	5.7	5.1	4.6	4.3	4.0	3.8	3.8
222	T	InChI=1S/C5H7N/c1-2-3-4-5-6/h2-3H,4H2,1H3/b3-2+	-0.6	0.6	1.0	1.0	0.8	0.6	0.4	0.2	0.1
223	T	InChI=1S/C5H7N/c1-3-4-5-6-2/h5H,1-2H3/b6-5+	-0.6	5.2	0.3	0.5	0.7	0.8	1.0	1.1	1.2
224	T	InChI=1S/C5H7N/c1-3-5(2)4-6/h2-3H2,1H3	-0.5	-0.8	0.3	0.5	0.5	0.5	0.4	0.3	0.1
225	T	InChI=1S/C5H7N/c1-3-5(2)4-6/h3H,1-2H3/b5-3-	-5.1	0.6	-0.7	-1.1	-1.1	-1.1	-0.8	-0.6	-0.4
226	T	InChI=1S/C5H7N/c1-3-5-6-4-2/h2-3,5-6H,1H3/b5-3+	4.2	2.8	-0.6	-0.4	-0.3	-0.3	-0.5	-0.6	-0.7
227	T	InChI=1S/C5H7N/c1-4-6-5(2)3/h1,6H,2H2,3H3	-3.2	-4.9	-0.4	-0.3	-0.2	0.0	0.4	0.7	0.9
228	T	InChI=1S/C5H7N/c1-5(2)3-4-6/h1,3H2,2H3	-1.8	-0.3	-1.8	-1.8	-1.6	-1.3	-0.8	-0.5	-0.3
229	T	InChI=1S/C5H7N/c1-5(2)3-4-6/h3H,1-2H3	-2.9	3.5	-1.1	-1.5	-1.5	-1.4	-1.0	-0.7	-0.4
230	T	InChI=1S/C5H8N/c1-3-5(2)4-6/h3H2,1-2H3	-1.3	3.7	-3.9	-2.4	-1.7	-1.3	-0.8	-0.6	-0.3
231	T	InChI=1S/C5H8N/c1-3-5-6-4-2/h3-4H,1-2H3	2.8	2.8	-2.2	-2.1	-1.8	-1.5	-1.0	-0.7	-0.2
232	T	InChI=1S/C5H8N/c1-4-6-5(2)3/h1,5H,2-3H3	-0.6	0.1	1.0	0.4	0.1	-0.1	-0.3	-0.3	-0.3
233	T	InChI=1S/C5H8N/c1-4-6-5(2)3/h4H,1-2H2,3H3	4.2	1.3	3.6	2.5	0.7	-0.6	-1.7	-1.8	-1.4

234	T	InChI=1S/C5H8N/c1-5(2)3-4-6/h5-6H,1-2H3	-1.5	-3.6	0.9	0.9	1.0	1.0	1.1	1.2	1.3
235	T	InChI=1S/C5H9N/c1-3-5(2)4-6/h5H,3H2,1-2H3/t5-/m0/s1	0.3	2.9	-0.9	-0.9	-0.8	-0.7	-0.5	-0.3	-0.2
236	T	InChI=1S/C5H9N/c1-3-5(6)4-2/h3-5H,1-2,6H2	-1.3	1.7	2.4	0.9	-0.2	-0.8	-1.0	-0.8	-0.4
237	T	InChI=1S/C5H9N/c1-3-5-6-4-2/h3,5H,1,4H2,2H3/b6-5-	-2.5	-3.1	1.6	2.5	2.9	2.8	2.3	1.8	1.1
238	T	InChI=1S/C5H9N/c1-3-5-6-4-2/h3-6H,2H2,1H3/b5-3+	1.9	0.6	1.5	1.3	1.0	1.0	1.2	1.4	1.4
239	T	InChI=1S/C5H9N/c1-4-6-5(2)3/h1,5-6H,2-3H3	-2.5	-4.7	-0.1	0.1	0.2	0.1	0.1	0.0	0.0
240	T	InChI=1S/C5H9N/c1-4-6-5(2)3/h4,6H,1-2H2,3H3	-3.2	-5.4	-2.7	-2.1	-1.0	-0.2	0.4	0.4	0.1
241	T	InChI=1S/C5H9N/c1-4-6-5(2)3/h4H,2H2,1,3H3/b6-4-	-0.6	-0.1	1.4	1.0	0.7	0.5	0.2	0.0	-0.1
242	T	InChI=1S/C5H9N/c1-5(2)3-4-6/h3-4,6H,1-2H3/b6-4-	-0.3	4.5	-1.2	-2.7	-3.3	-3.3	-2.8	-2.1	-1.1
243	T	InChI=1S/C5H9N/c1-5(2,3)4-6/h1-3H3	0.6	5.2	-1.7	-2.3	-2.3	-2.0	-1.5	-1.1	-0.5
244	T	InChI=1S/C6H11N/c1-3-5-6(7)4-2/h3-6H,2,7H2,1H3/b5-3-/t6-/m0/s1	3.6	1.8	-0.6	-1.8	-1.9	-1.6	-1.0	-0.7	-0.4
245	T	InChI=1S/C6H11N/c1-3-6(2)4-5-7/h4-5,7H,3H2,1-2H3/b6-4+,7-5+	0.2	-1.5	-2.3	-3.1	-2.9	-2.3	-1.4	-0.9	-0.3
246	T	InChI=1S/C6H11N/c1-3-6(4-2)5-7/h6H,3-4H2,1-2H3	-1.3	-0.4	0.2	0.0	-0.1	-0.1	0.0	0.0	0.0
247	T	InChI=1S/C6H11N/c1-4-6(2,3)5-7/h4H2,1-3H3	0.3	4.9	-3.0	-3.0	-2.5	-2.1	-1.4	-1.0	-0.5
248	T	InChI=1S/C6H11N/c1-4-6(5-2)7-3/h4-7H,1-2H2,3H3	-2.3	-3.5	-1.7	0.9	2.1	2.4	2.0	1.5	0.8
249	T	InChI=1S/C6H11N/c1-5(2)7-6(3)4/h7H,1,3H2,2,4H3	6.0	3.1	-1.9	-2.3	-2.7	-3.0	-3.8	-4.1	-3.8
250	T	InChI=1S/C6H11N/c1-6(2)4-5-7-3/h4-5H,1-3H3/b7-5-	-1.2	2.9	0.6	-1.2	-2.0	-2.3	-2.0	-1.6	-0.9
251	T	InChI=1S/C6H11NO2/c1-3-5-6(4-2)9-7-8/h3,6H,1,4-5H2,2H3/t6-/m0/s1	-2.0	-2.8	6.6	7.6	8.3	8.7	8.7	8.3	7.0
252	T	InChI=1S/C6H13N/c1-5-6(2,3)7-4/h5,7H,1H2,2-4H3	3.6	-2.8	1.6	1.6	1.4	1.2	0.8	0.5	0.1
253	T	InChI=1S/C6H13N/c1-5-7(4)6(2)3/h5-6H,1H2,2-4H3	3.6	-6.4	0.1	1.0	1.0	0.5	-0.2	-0.6	-0.5
254	T	InChI=1S/C6H13NO/c1-4-5-6(8)7(2)3/h4-5H2,1-3H3	1.3	-5.8	-0.9	-0.3	0.1	0.3	0.5	0.6	0.7
255	T	InChI=1S/C6H13NO/c1-4-7(5-2)6(3)8/h4-5H2,1-3H3	0.2	-5.6	3.1	4.0	4.2	4.0	3.0	2.1	0.7
256	T	InChI=1S/C6H15N/c1-3-5-7-6-4-2/h7H,3-6H2,1-2H3	0.0	0.8	-3.4	-3.2	-2.8	-2.4	-1.7	-1.1	-0.4
257	T	InChI=1S/C6H15N/c1-4-7(5-2)6-3/h4-6H2,1-3H3	0.6	-1.0	0.5	0.2	0.2	0.2	0.2	0.2	0.2
258	T	InChI=1S/C6H15N/c1-5(2)7-6(3)4/h5-7H,1-4H3	2.7	3.2	-1.3	-0.9	0.0	0.8	1.6	1.6	0.7
259	T	InChI=1S/C6H6N/c1-3-5-7-6-4-2/h1-2H3	-0.3	5.9	1.8	1.6	1.6	1.7	1.8	1.9	2.1
260	T	InChI=1S/C6H7N/c1-6(2)4-3-5-7/h6H,1-2H3	-0.9	0.0	0.2	0.1	-0.1	-0.1	-0.2	-0.2	-0.1
261	T	InChI=1S/C6H8N/c1-3-4-6(2)5-7/h3H,1,4H2,2H3	1.4	-6.1	4.7	3.2	2.3	1.7	1.0	0.6	0.1
262	T	InChI=1S/C6H8N/c1-6(2)4-3-5-7/h3-4H,1-2H3	-3.5	3.3	-4.1	-4.3	-3.8	-3.2	-2.2	-1.5	-0.8
263	T	InChI=1S/C6H9N/c1-3-6(2)4-5-7/h4H,3H2,1-2H3/b6-4+	-2.7	-2.7	-0.9	-0.5	-0.2	-0.1	0.0	0.0	-0.1
264	T	InChI=1S/C7H11N/c1-3-5-7(4-2)6-8/h3,7H,1,4-5H2,2H3/t7-/m1/s1	-1.0	-6.8	2.1	2.2	2.0	1.8	1.3	0.9	0.4
265	T	InChI=1S/C7H11N/c1-4-5-7(2,3)6-8/h4H,1,5H2,2-3H3	-1.0	-7.0	5.2	4.0	3.5	3.1	2.4	1.8	0.8

266	T	InChI=1S/C7H13N/c1-4-5-7(2,3)6-8/h4-5H2,1-3H3	0.1	-3.1	-0.5	1.2	1.3	1.0	0.5	0.3	0.2
267	T	InChI=1S/C7H14N/c1-4-7(3)6-8-5-2/h6H,4-5H2,1-3H3	-3.4	-5.3	-0.6	-0.4	-0.2	0.0	0.2	0.2	0.2
268	T	InChI=1S/C7H17N/c1-4-5-8-6-7(2)3/h7-8H,4-6H2,1-3H3	0.9	4.0	-0.8	-0.6	-0.4	-0.1	0.2	0.3	-0.3
269	T	InChI=1S/C8H19N/c1-3-5-7-9-8-6-4-2/h9H,3-8H2,1-2H3	1.4	7.3	-1.9	-2.4	-2.4	-2.2	-1.7	-1.1	-0.5
270	T	InChI=1S/CH2N/c1-2/h1-2H	-2.4	-4.3	2.1	2.3	2.1	1.9	1.5	1.2	0.8
271	T	InChI=1S/CH2N/c1-2/h1H2	-5.2	-6.3	0.4	-0.1	-0.1	0.0	0.4	0.6	0.6
272	T	InChI=1S/CH3N/c1-2/h2H,1H2	1.7	0.4	-0.6	-1.2	-1.3	-1.2	-0.7	-0.4	-0.2
273	T	InChI=1S/CH3NO/c1-2-3/h1H3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
274	T	InChI=1S/CH3NO2/c1-2(3)4/h1H3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
275	T	InChI=1S/CH3NO2/c1-4-2-3/h1H3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
276	T	InChI=1S/CH4N/c1-2/h1-2H2	2.8	-5.8	2.6	2.6	2.7	2.7	2.4	2.0	1.2
277	T	InChI=1S/CH4N/c1-2/h2H,1H3	-2.5	-3.2	3.8	2.9	2.2	1.8	1.3	1.1	0.8
278	T	InChI=1S/CH4NO/c1-2-3/h2H,1H3	1.8	-4.2	3.5	3.5	3.0	2.4	1.6	1.2	0.7
279	T	InChI=1S/CH4NO/c1-2-3/h3H,1H3	-1.5	-1.5	1.0	0.8	0.8	0.8	0.8	0.7	0.5
280	T	InChI=1S/CH5N/c1-2/h2H2,1H3	-0.5	-1.7	3.4	2.0	1.1	0.7	0.3	0.2	0.2
281	T	InChI=1S/CH6N2/c1-3-2/h3H,2H2,1H3	0.8	-0.3	0.3	0.1	-0.2	-0.4	-0.5	-0.5	-0.1
282	V	InChI=1S/C3H8N2/c1-2-3(4)5/h2H,4-5H2,1H3	-1.6	-1.9	4.5	3.8	2.1	0.6	-0.9	-0.9	0.1
283	V	InChI=1S/C4H10N/c1-2-3-4-5/h5H,2-4H2,1H3	2.5	0.3	-2.0	-1.1	-0.6	-0.4	-0.3	-0.2	-0.2
284	V	InChI=1S/C4H10N2/c1-2-3-6-4-5/h2,6H,1,3-5H2	-0.1	-0.7	-0.2	0.1	0.3	0.4	0.3	0.2	0.0
285	V	InChI=1S/C4H10NO/c1-3-5(6)4-2/h3-4H2,1-2H3	-1.5	1.7	-4.0	-3.6	-2.9	-2.3	-1.4	-1.0	-0.5
286	V	InChI=1S/C4H8N/c1-3-4(2)5/h5H,2-3H2,1H3	1.6	-2.5	-0.6	-0.5	-0.4	-0.4	-0.4	-0.4	-0.2
287	V	InChI=1S/C5H10N/c1-5(2)4-6-3/h4-5H,3H2,1-2H3	1.6	2.3	0.2	-0.2	-0.3	-0.4	-0.3	-0.3	-0.5
288	V	InChI=1S/C5H11N/c1-3-4-5(2)6/h4H,3,6H2,1-2H3/b5-4-	0.5	-2.6	-3.6	-2.4	-1.2	-0.4	0.3	0.3	0.1
289	V	InChI=1S/C5H11N/c1-3-5-6-4-2/h5H,3-4H2,1-2H3/b6-5-	1.9	-1.8	-0.6	-0.1	0.0	0.1	0.0	-0.1	-0.1
290	V	InChI=1S/C5H11NO2/c1-3-5(4-2)8-6-7/h5H,3-4H2,1-2H3	-0.9	-3.0	-1.9	-1.7	-1.3	-1.1	-1.2	-1.5	-1.7
291	V	InChI=1S/C5H12N2/c1-3-4-5(6)7-2/h3-5,7H,6H2,1-2H3/b4-3+/t5-/m1/s1	-2.1	-2.1	-0.4	0.8	2.1	3.0	3.4	2.9	1.5
292	V	InChI=1S/C5H12N2/c1-3-4-5-7-6-2/h3-5H2,1-2H3	0.2	-2.5	-0.8	0.2	0.6	0.6	0.5	0.4	0.2
293	V	InChI=1S/C5H8N/c1-5(2)3-4-6/h3,5H,1-2H3	1.0	-0.2	-0.1	-0.5	-0.6	-0.6	-0.6	-0.7	-0.6
294	V	InChI=1S/C6H11N/c1-4-5-7-6(2)3/h5H,2,4H2,1,3H3/b7-5+	-1.3	0.7	0.1	-0.2	-0.4	-0.4	-0.4	-0.2	-0.1
295	V	InChI=1S/C6H13N/c1-4-5-6(2,3)7/h4-5H,7H2,1-3H3/b5-4+	-2.2	2.5	-1.1	-1.0	-0.9	-0.8	-0.5	-0.3	-0.1
296	V	InChI=1S/C6H13NO/c1-4-6(8)7(3)5-2/h4-5H2,1-3H3	-0.1	3.1	-2.4	-1.1	-0.4	0.1	0.6	0.7	0.7
297	V	InChI=1S/C6H13NO2/c1-4-6(2,3)5-7(8)9/h4-5H2,1-3H3	2.7	-3.1	6.6	5.2	3.9	2.9	1.5	0.7	-0.5

298	V	InChI=1S/C6H14N/c1-4-6(2,3)5-7/h5H,4,7H2,1-3H3	-2.6	2.3	2.6	3.1	2.6	1.9	0.8	0.2	-0.2
299	V	InChI=1S/C6H15N/c1-4-6(2,3)5-7/h4-5,7H2,1-3H3	2.3	2.6	1.8	1.6	1.3	0.9	0.4	0.0	-0.3
300	V	InChI=1S/C6H8N2/c7-5-3-1-2-4-6-8/h1-4H2	1.1	-0.3	1.8	1.6	1.2	0.8	0.5	0.3	0.2

4. Comparison with previously derived GAVs

Table S4: Differences between group additive values for the standard enthalpy of formation [kJ mol⁻¹], the standard entropy and heat capacity [J mol⁻¹ K⁻¹] at different temperatures for nitrogen-containing compounds obtained in this work and reported by Benson et al. [4] for all groups in common.

Group	GAV (current work) – GAV(literature)								
	$\Delta_f H^\circ$	S°	C_p°						
	298 K	298 K	300 K	400 K	500 K	600 K	800 K	1000 K	1500 K
C-(C)(N)(H) ₂	-0.2	-3.6	3.7	2.5	1.7	1.3	0.8	0.6	
C-(C)(CN)(H) ₂	3.9	-2.2	2.6	2.1	0.8	-0.2	-1.1	-0.7	
C-(C)(N _A)(H) ₂	-3.9	1.3	-	-	-	-	-	-	-
C-(N) ₂ (H) ₂	3.7	-	-	-	-	-	-	-	-
C-(C) ₂ (N)(H)	3.1	-3.0	5.5	4.2	2.7	2.6	1.5	1.2	-
C-(C) ₂ (CN)(H)	4.0	-8.0	2.7	3.9	4.4	3.9	2.9	2.2	-
C-(C) ₃ (N)	1.3	-0.5	5.5	4.4	3.0	2.2	0.6	0.4	-
C _d -(CN)(H)	-7.2	4.8	0.0	-0.8	-1.3	-1.2	-1.0	0.3	-
C _t -(CN)	-21.3	-3.0	-1.0	-0.8	-1.0	-0.9	-0.7	-0.6	-0.6
CO-(C)(N)	15.8	-10.6	-1.9	0.3	1.0	2.1	-1.3	-5.1	
C-(C)(NO)(H) ₂	8.8	-	-	-	-	-	-	-	-
C-(C) ₂ (NO)(H)	4.1	-	-	-	-	-	-	-	-
C-(C)(NO ₂)(H) ₂	-2.1	0.4	-	-	-	-	-	-	-
C-(C) ₂ (NO ₂)(H)	5.8	-1.8	-	-	-	-	-	-	-
N-(CO)(H) ₂	-10.0	19.6	11.2	6.9	3.6	1.4	-0.7	-1.6	-
N-(C)(CO)(H)	-9.7	-	-	-	-	-	-	-	-
N-(C)(H) ₂	1.1	0.8	-2.8	-1.6	-0.8	-0.3	-0.1	0.0	0.1
N-(C) ₂ (H)	5.6	-1.5	2.7	1.3	0.6	0.3	0.0	-0.3	0.0
N-(C) ₃	0.0	1.6	0.7	0.6	0.7	1.1	1.5	1.9	2.4
N-(N)(H) ₂	-1.4	1.4	0.7	0.3	-0.3	-0.8	-1.5	-2.0	-2.5
N-(C)(N)(H)	4.1	-8.4	1.1	0.8	1.1	1.5	1.9	2.4	3.4
N-(C) ₂ (N)	1.2	0.2	-	-	-	-	-	-	-
N _t -(C)	7.9	-	-	-	-	-	-	-	-
N _A -(C)	-14.1	-	-	-	-	-	-	-	-

Table S5: Differences between group additive values and pairs of linear dependent for the standard enthalpy of formation [kJ mol⁻¹] for nitrogen-containing compounds obtained in this work and reported by Holmes and Aubry [5] for all groups in common.

Group	GAV (current work) – GAV (literature)	Pairs of linear dependent groups	GAVs (current work) – GAVs (literature)
	$\Delta_f H^\circ$		$\Delta_f H^\circ$
C-(C)(N)(H) ₂	-4.8	C-(CN)(C)(H) ₂ +CN-(C)	4.1
C-(C)(CN)(H) ₂	124.1	C-(CN)(C _d)(H) ₂ +CN-(C _d)	9.1
C-(C _d)(CN)(H) ₂	124.1	N-(CO)(H) ₂ +CO-(N)(C)	2.1
C-(C) ₂ (N)(H)	-0.6	N-(C)(CO)(H)+CO-(N)(C)	6.4
C-(C) ₃ (N)	0.9		
C _d -(C)(N)	0.4		
C ₁ -(C)(H)	26		
C ₁ -(C _d)(H)	3.0		
C ₁ -(C) ₂	3.5		
N-(CO)(H) ₂	39		
N-(C)(CO)(H)	-8.1		
N-(C) ₂ (CO)	1.0		
N-(C)(H) ₂	3.1		
N-(C) ₂ (H)	5.0		
N-(C) ₃	0.0		
N-(C)(C _d)(H)	-3.2		
N-(C _d) ₂ (H)	-1.6		
N ₁ -(H)	-2.3		
N ₁ -(C)	1.0		
N ₁ -(C _d)	-12.9		

Table S6: Differences between group additive values and pairs of linear dependent groups for the standard enthalpy of formation [kJ mol⁻¹], the standard entropy and heat capacity [J mol⁻¹ K⁻¹] at different temperatures for nitrogen-containing compounds obtained in this work and reported by Ashcraft et al. [6] for all groups in common.

Group	GAV (current work) – GAV(literature)								
	$\Delta_f H^\circ$	S°	C_p°						
	298 K	298 K	300 K	400 K	500 K	600 K	800 K	1000 K	1500 K
C-(C)(N)(H) ₂	-0.2	-3.6	3.5	2.5	1.6	1.2	0.7	0.7	-1.9
C-(C)(C ₁)(H) ₂	1.6	0.1	0.5	0.3	0.3	0.1	-0.2	-0.4	-0.1
C-(C)(CN)(H) ₂	2.3	-0.5	1.7	1.7	1.6	1.4	1.0	1.0	1.1
C-(C)(N _A)(H) ₂	-3.9	3.0	0.2	-0.1	-0.5	-0.5	-0.7	-0.5	-0.3
C-(C) ₂ (C ₁)(H)	1.8	0.2	0.6	0.2	0.2	0.5	0.1	0.5	0.6
C-(C) ₃ (CN)	4.2	-6.0	2.8	3.3	3.6	3.9	3.2	3.3	3.2
C _d -(C)(N)	26.7	0.9	-1.7	-3.5	-3.9	-3.8	-3.3	-2.3	-
C _d -(C)(CN)	-2.7	-3.1	3.1	2.9	2.6	2.7	2.2	1.8	1.3
C ₁ -(C)(H)	10.1	-6.2	-5.6	-5.5	-5.7	-6.1	-6.3	-7.2	-
C ₁ -(C) ₂	1.6	-54.9	-1.5	-1.8	-2.6	-3.2	-4.4	-5.0	-6.0
C-(C)(NO)(H) ₂	-0.9	-1.4	-1.0	-0.9	-0.4	-0.4	0.1	0.3	0.2
C-(C) ₂ (NO)(H)	-0.9	-7.2	5.2	4.5	3.9	3.4	2.5	2.3	1.9
C-(C)(NO ₂)(H) ₂	-3.4	-1.7	3.0	2.2	1.7	1.5	1.1	0.7	0.2
C-(C) ₂ (NO ₂)(H)	-2.2	-4.3	0.6	0.9	1.4	1.9	2.1	2.1	1.8
N-(C _d)(H) ₂	-27.0	-0.6	2.0	2.4	2.0	1.8	1.7	1.4	1.2
N-(C)(C _d)(H)	-26.2	0.0	-2.7	-1.8	-0.9	0.5	1.7	2.5	2.8
N-(N)(H) ₂	-1.4	1.5	0.7	0.2	-0.2	-0.9	-1.4	-1.9	-2.5
N-(C)(N)(H)	4.1	-8.3	1.2	0.8	1.1	1.5	1.9	2.4	3.4
N-(C) ₂ (N)	11.2	3.1	-0.2	-1.5	-2.0	-1.7	-0.7	0.6	1.7
N ₁ -(H)	-6.5	55.1	5.2	5.0	5.4	5.9	6.6	7.2	8.0
N ₁ -(C)	7.9	56.7	6.6	5.7	6.4	7.0	8.3	8.7	9.7
N _A -(C)	8.9	-1.7	-0.1	0.1	0.8	1.1	1.2	1.0	1.1
Pairs of linear dependent GAVs									
N-(C _d)(H) ₂ + C _d -(C)(N)	-0.3	-0.6	2.0	2.4	2.0	1.8	1.7	1.4	1.2
N-(C _d)(C)(H) + C _d -(C)(N)	0.5	0.0	-2.7	-1.8	-0.9	0.5	1.7	2.5	2.8

References

- [1] B. Ruscic, D.H. Bross, Active Thermochemical Tables (ATcT) values based on ver. 1.122d of the Thermochemical Network (2018); available at ATcT.anl.gov, 2018.
- [2] J. Pedley, R.D. Naylor, S.P. Kirby, Thermochemical data of organic compounds, Springer Netherlands, 1986.
- [3] P.J. Lindstrom, W.G. Mallard, NIST Chemistry WebBook, NIST Standard Reference Database Number 69, National Institute of Standards and Technology, Gaithersburg MD.
- [4] S.W. Benson, F.R. Cruickshank, D.M. Golden, G.R. Haugen, H.E. O'Neal, A.S. Rodgers, R. Shaw, R. Walsh, Additivity rules for the estimation of thermochemical properties, Chemical Reviews 69 (1969) 279-324.
- [5] J.L. Holmes, C. Aubry, Group Additivity Values for Estimating the Enthalpy of Formation of Organic Compounds: An Update and Reappraisal. 2. C, H, N, O, S, and Halogens, The Journal of Physical Chemistry A 116 (2012) 7196-7209.
- [6] R.W. Ashcraft, W.H. Green, Thermochemical Properties and Group Values for Nitrogen-Containing Molecules, The Journal of Physical Chemistry A 112 (2008) 9144-9152.