Enthalpies of Formation of Hydrazine and Its Derivatives

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Supporting Information

Content

Table S1. Experimental Enthalpies of Formation of Reference Compounds Used in Isodesmic Reactions

compound		$\Delta_f H^\circ_{298}$(g), kJ/mol	reference
CH_2N_4	1*H*-tetrazole	327.2 ± 1.8	1
CH_3NO	$CH_3N{=}O$	69.9 ± 3.0	2
CH_3NO	$HC(O)NH_2$	-188.6 ± 0.4	3
CH_3NO_2	CH_3NO_2	-71.5 ± 0.4	4
CH_3N_5	5-amino-1*H*-tetrazole	323.8 ± 2.6	1
CH_4N_2O	$H_2NC(O)NH_2$	-235.5 ± 1.2	5
$CH_4N_2O_2$	CH_3NHNO_2	1.3 ± 0.4	6
CH_4N_2S	$H_2NC(S)NH_2$	22.9 ± 1.6	7
CH_4S	CH_3SH	-22.9 ± 0.6	8
CH_5N_3S	$H_2NC(S)NHNH_2$	128.2 ± 1.6	7
$C_2H_2N_4$	1,2,4,5-tetrazine	478.7 ± 4.0	9
$C_2H_2O_4$	$HOC(O)C(O)OH$	-732.0 ± 3.0	10, 11
C_2H_3N	CH_3CN	74.0 ± 0.3	8
$C_2H_4N_2O_2$	$H_2NC(O)C(O)NH_2$	-387.1 ± 1.3	8
$C_2H_4N_4$	5-methyl-1*H*-tetrazole	280.7 ± 2.6	1
$C_2H_4N_4O_4$	FOX-7: $(O_2N)_2C{=}C(NH_2)_2$	3.4 ± 8.0	12
C_2H_5NO	$CH_3C(O)NH_2$	-237.1 ± 0.8	13, 14
$C_2H_5NO_2$	$CH_3CH_2NO_2$	-102.5 ± 0.8	15, 16
$C_2H_5NO_2$	$H_2NCH_2C(O)OH$ (Gly)	-393.7 ± 1.5	17, 18
$C_2H_5N_5$	1-methyl-5-amino-1*H*-tetrazole	302.4 ± 2.8	1
$C_2H_6N_2O_2$	$CH_3N(NO_2)CH_3$	-7.5 ± 2.1	19
$C_2H_6O_2$	CH_3OOCH_3	-125.7 ± 1.2	8
C_2H_6S	CH_3CH_2SH	-46.1 ± 0.6	8
C_2H_6S	CH_3SCH_3	-37.4 ± 0.6	8
C_2H_7N	$CH_3CH_2NH_2$	-47.5 ± 0.6	8
$C_2H_8N_2$	$H_2NCH_2CH_2NH_2$	-18.0 ± 0.7	8
$C_3H_4N_2$	1*H*-pyrazole	179.4 ± 0.8	20
$C_3H_4N_2$	1*H*-imidazole	132.9 ± 0.6	20
$C_3H_6N_2O$	imidazolidin-2-one	-176.7 ± 2.2	21
$C_3H_7NO_2$	$CH_3CH(NH_2)C(O)OH$ (Ala)	-424.8 ± 2.0	17, 18
$C_3H_7NO_2$	$H_2NCH_2CH_2C(O)OH$ (β-Ala)	-421.2 ± 1.9	22
$C_4H_2N_6O_4$	DNPP: 3,6-dinitropyrazolo[4,3-c]pyrazole	407.2 ± 4.0	9
$C_4H_4N_2$	pyridazine	280.2 ± 0.7	23
$C_4H_4N_2$	pyrimidine	189.7 ± 0.7	23
$C_4H_4N_2$	pyrazine	203.2 ± 1.5	23
$C_4H_4N_2O_2$	uracil	-303.1 ± 2.3	24
C_4H_4O	furan	-34.8 ± 0.7	8
$C_4H_6N_2O_2$	5,6-dihydrouracil	-377.2 ± 1.6	25
C_4H_8O	$CH_3C(O)CH_2CH_3$	-238.5 ± 0.9	8
$C_4H_8O_2$	$(CH_3)_2CHC(O)OH$	-476.6 ± 1.0	26
$C_4H_8O_2$	$CH_3C(O)OCH_2CH_3$	-444.6	27
$C_4H_{10}O$	$CH_3CH_2CH_2CH_2OH$	-274.9 ± 0.4	8
$C_4H_{10}O$	$CH_3CH_2OCH_2CH_3$	-252.2 ± 0.8	28
$C_4H_{11}N$	$CH_3CH_2NHCH_2CH_3$	-72.2 ± 1.2	8
$C_5H_4O_2$	3-furaldehyde	-151.9 ± 1.1	29
C_5H_5N	pyridine	140.4 ± 0.7	8
$C_5H_6N_2$	4-aminopyridine	129.9 ± 1.4	8
$C_5H_6N_2O_2$	2-furancarboxylic acid hydrazide	-106.5 ± 1.1	30
$C_5H_7NO_2$	glutarimide	-393.6 ± 1.8	31
C_5H_{10}	$CH_3CH{=}C(CH_3)_2$	-41.0 ± 1.3	32, 33
C_5H_{12}	$(CH_3)_2CHCH_2CH_3$	-153.6 ± 0.9	8
$C_6H_4N_2O$	benzofurazan	300.2 ± 2.1	34
$C_6H_5NO_2$	$C_6H_5NO_2$	65.6 ± 1.6	4
$C_6H_5NO_2$	4-pyridinecarboxylic acid	-234.8 ± 4.7	35

$C_6H_6N_2O$	2-pyridinecarboxamide	-63.3 ± 3.8	36
C_6H_6O	C_6H_5OH	-91.8 ± 2.5	37
$C_6H_6O_2$	2-acetylfuran	-207.4 ± 1.3	29
C_6H_7N	$C_6H_5NH_2$	87.1 ± 1.1	8
$C_6H_8N_2$	5,6-dimethyluracil	-376.2 ± 2.6	38
C_6H_{14}	$(CH_3)_2CHCH(CH_3)_2$	-178.1 ± 0.9	8
$C_7H_6N_2$	1*H*-indazole	243.0 ± 1.3	20
$C_7H_6N_2$	1*H*-benzimidazole	181.7 ± 1.4	20
$C_7H_6N_2O$	2-benzimidazolinone	-63.9 ± 2.9	39
$C_7H_6N_2O$	3-indazolinone	70.0 ± 2.2	39
$C_7H_6N_4$	5-phenyl-1*H*-tetrazole	413.0 ± 5.9	40
C_7H_6O	$C_6H_5C(O)H$	-36.7 ± 2.8	8
$C_7H_6O_2$	$C_6H_5C(O)OH$	-294.0 ± 2.2	8
C_7H_7NO	$C_6H_5C(O)NH_2$	-99.0 ± 1.2	41, 42
C_7H_8O	$C_6H_5CH_2OH$	-94.6 ± 3.0	43
C_7H_8O	$C_6H_5OCH_3$	-70.7 ± 1.4	44
C_7H_9N	$C_6H_5CH_2NH_2$	86.2 ± 1.8	45
C_7H_9N	$C_6H_5NHCH_3$	90.9 ± 2.1	46
C_8H_8	$C_6H_5CH=CH_2$	148.0 ± 1.4	8
C_8H_8O	$C_6H_5C(O)CH_3$	-86.7 ± 1.5	8
C_8H_{10}	$C_6H_5CH_2CH_3$	29.9 ± 0.4	47
$C_8H_{11}N$	$C_6H_5NHCH_2CH_3$	66.5 ± 1.1	48
$C_8H_{11}N$	$C_6H_5N(CH_3)_2$	100.0 ± 1.0	48
$C_8H_{11}N$	2,4-dimethylaniline	23.2 ± 1.0	48
C_9H_8	indene	161.2 ± 2.3	49
C_9H_{10}	indane	60.9 ± 2.1	49
C_9H_{12}	$C_6H_5CH(CH_3)_2$	4.0 ± 1.0	8
C_9H_{12}	1,3,5-trimethylbenzene	-15.9 ± 1.3	8
$C_9H_{13}N$	1,4-CH_3-C_6H_4-$N(CH_3)_2$	68.9 ± 7.4	50
$C_{10}H_{14}$	$C_6H_5C(CH_3)_3$	-24.4 ± 0.8	51
$C_{13}H_{10}O$	$C_6H_5C(O)C_6H_5$	50.9 ± 2.4	52
H_2S	H_2S	-20.6 ± 0.5	53

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Table S2. Enthalpies of Formation of Hydrazine and Its Derivatives Calculated from Atomization, Isodesmic, Isogyric, and other Balanced Reactions Using G4 Energies (in kJ/mol)[a]

	reaction	$\Delta_f H^\circ_{298}$ kJ/mol
	hydrazine: NH_2NH_2	
	atomization reaction	100.3
	reactions with radicals from ATcT	
1	$NH_2NH_2 + 2\ {\bullet}CH_3 \rightarrow 2\ {\bullet}NH_2 + CH_3CH_3$	96.5
2	$NH_2NH_2 + {\bullet}CH_3 \rightarrow {\bullet}NH_2 + CH_3NH_2$	97.5
3	$NH_2NH_2 + {\bullet}CH_2CH_3 \rightarrow {\bullet}NH_2 + CH_3NHCH_3$	100.5
4	$NH_2NH_2 + {\bullet}H \rightarrow {\bullet}NH_2 + NH_3$	97.7
5	$NH_2NH_2 + {\bullet}OH \rightarrow {\bullet}NH_2 + NH_2OH$	97.2
6	$NH_2NH_2 + {\bullet}C(O)OH \rightarrow {\bullet}NH_2 + NH_2OH + CO$	96.8
7	$NH_2NH_2 + {\bullet}C(O)H \rightarrow {\bullet}NH_2 + NH_3 + CO$	96.3
	average of 7 reactions with $\bullet NH_2$	**97.5**
8	$NH_2NH_2 + 2\ {\bullet}CH_3 \rightarrow 2\ {\bullet}CH_2NH_2 + H_2$	95.3
9	$NH_2NH_2 + {\bullet}CH_3 \rightarrow {\bullet}CH_2NH_2 + NH_3$	94.3
10	$NH_2NH_2 + {\bullet}CH_2CH_3 \rightarrow {\bullet}CH_2NH_2 + CH_3NH_2$	97.8
11	$NH_2NH_2 + {\bullet}CH(CH_3)_2 \rightarrow {\bullet}CH_2NH_2 + CH_3NHCH_3$	97.7
12	$NH_2NH_2 + {\bullet}CH_2OH \rightarrow {\bullet}CH_2NH_2 + NH_2OH$	96.2
13	$NH_2NH_2 + CH_3O{\bullet} \rightarrow {\bullet}CH_2NH_2 + NH_2OH$	92.8
14	$NH_2NH_2 + {\bullet}CH_2C(O)H \rightarrow {\bullet}CH_2NH_2 + NH_3 + CO$	94.7
	average of 7 reactions with $\bullet CH_2NH_2$	**95.5**
15	$NH_2NH_2 + 2\ {\bullet}CH_3 \rightarrow 2\ {\bullet}NHCH_3 + H_2$	98.9
16	$NH_2NH_2 + {\bullet}CH_3 \rightarrow {\bullet}NHCH_3 + NH_3$	96.1
17	$NH_2NH_2 + {\bullet}CH_2CH_3 \rightarrow {\bullet}NHCH_3 + CH_3NH_2$	99.6
18	$NH_2NH_2 + {\bullet}CH(CH_3)_2 \rightarrow {\bullet}NHCH_3 + CH_3NHCH_3$	99.5
19	$NH_2NH_2 + {\bullet}CH_2OH \rightarrow {\bullet}NHCH_3 + NH_2OH$	98.0
20	$NH_2NH_2 + CH_3O{\bullet} \rightarrow {\bullet}NHCH_3 + NH_2OH$	94.6
21	$NH_2NH_2 + {\bullet}CH_2C(O)H \rightarrow {\bullet}NHCH_3 + NH_3 + CO$	96.6
	average of 7 reactions with $\bullet NHCH_3$	**97.6**
22	$NH_2NH_2 + {\bullet}CH_3 \rightarrow {\bullet}NHNH_2 + CH_4$	97.6
23	$NH_2NH_2 + {\bullet}CH_2CH_3 \rightarrow {\bullet}NHNH_2 + CH_3CH_3$	98.9
24	$NH_2NH_2 + {\bullet}OH \rightarrow {\bullet}NHNH_2 + H_2O$	96.3
25	$NH_2NH_2 + {\bullet}OOH \rightarrow {\bullet}NHNH_2 + H_2O_2$	96.7
26	$NH_2NH_2 + {\bullet}NH_2 \rightarrow {\bullet}NHNH_2 + NH_3$	96.4
27	$NH_2NH_2 + {\bullet}C_6H_5 \rightarrow {\bullet}NHNH_2 + C_6H_6$	98.3
28	$NH_2NH_2 + CH_3O{\bullet} \rightarrow {\bullet}NHNH_2 + CH_3OH$	95.6
	average of 7 reactions with $\bullet NHNH_2$	**97.1**
29	$NH_2NH_2 + {\bullet}OH \rightarrow {\bullet}NHOH + NH_3$	96.4
30	$NH_2NH_2 + {\bullet}OOH \rightarrow {\bullet}NHOH + NH_2OH$	98.8
31	$NH_2NH_2 + CH_3O{\bullet} \rightarrow {\bullet}NHOH + CH_3NH_2$	95.2
32	$NH_2NH_2 + {\bullet}CH_2OH \rightarrow {\bullet}NHOH + CH_3NH_2$	98.6
33	$NH_2NH_2 + CH_3CH_2O{\bullet} \rightarrow {\bullet}NHOH + CH_3NHCH_3$	96.8
34	$NH_2NH_2 + {\bullet}CH_2CH_2OH \rightarrow {\bullet}NHOH + CH_3NHCH_3$	98.5
35	$NH_2NH_2 + {\bullet}C(O)OH \rightarrow {\bullet}NHOH + CO + NH_3$	96.0
	average of 7 reactions with $\bullet NHOH$	**97.2**
	average of 35 reactions (1-35) with radicals	**97.0**

reactions with species from ATcT

36	$NH_2NH_2 + H_2 \rightarrow 2\ NH_3$	93.3
37	$NH_2NH_2 + CH_4 \rightarrow CH_3NH_2 + NH_3$	96.2
38	$NH_2NH_2 + CH_3CH_3 \rightarrow 2\ CH_3NH_2$	98.4
39	$NH_2NH_2 + CH_3CH_3 \rightarrow CH_3NHCH_3 + NH_3$	98.0
40	$NH_2NH_2 + CH_3CH_3 \rightarrow CH_2{=}CH_2 + 2\ NH_3$	93.0
41	$NH_2NH_2 + CH_3CH_3 \rightarrow HN{=}NH + 2\ CH_4$	98.9
42	$NH_2NH_2 + H_2C{=}CH_2 \rightarrow HN{=}NH + CH_3CH_3$	100.0
43	$NH_2NH_2 \rightarrow HN{=}NH + H_2$	99.7
44	$NH_2NH_2 + H_2O \rightarrow NH_2OH + NH_3$	97.3
45	$NH_2NH_2 + HOOH \rightarrow 2\ NH_2OH$	99.2
46	$NH_2NH_2 + CH_3OH \rightarrow NH_2OH + CH_3NH_2$	96.7
47	$NH_2NH_2 + CH_3CH_2OH \rightarrow CH_3NHCH_3 + NH_2OH$	99.7
48	$NH_2NH_2 + CH_3OCH_3 \rightarrow CH_3NHCH_3 + NH_2OH$	97.3
49	$NH_2NH_2 + CH_3OCH_3 \rightarrow CH_3OH + CH_2NH + NH_3$	95.8
50	$NH_2NH_2 + HOCH_2CH_2OH \rightarrow 2\ NH_2OH + H_2C{=}CH_2$	94.8
51	$NH_2NH_2 + HC(O)H \rightarrow 2\ NH_3 + CO$	93.3
52	$NH_2NH_2 + 2\ HC(O)OH \rightarrow 2\ NH_2OH + HC(O)C(O)H$	99.6
53	$NH_2NH_2 + HCN \rightarrow NH_2CN + NH_3$	96.0
54	$NH_2NH_2 + NCCN \rightarrow 2\ NH_2CN$	93.6
55	$NH_2NH_2 + HOCN \rightarrow NH_2OH + NH_2CN$	96.3
	average of 20 reactions (36-55) with species from ATcT	**96.9**

reactions with species not from ATcT

56	$NH_2NH_2 + CH_3CH_3 \rightarrow CH_3CH_2NH_2 + NH_3$	97.8
57	$NH_2NH_2 + CH_3CH_2CH_2CH_3 \rightarrow H_2NCH_2CH_2NH_2 + CH_3CH_3$	98.7
58	$NH_2NH_2 + C_6H_5CH_3 \rightarrow C_6H_5NH_2 + CH_3NH_2$	98.7
59	$NH_2NH_2 + C_6H_5CH_3 \rightarrow C_6H_5CH_2NH_2 + NH_3$	96.6
60	$NH_2NH_2 + CH_3OCH_3 \rightarrow CH_3CH_2NH_2 + NH_2OH$	97.2
61	$NH_2NH_2 + C_6H_5OH \rightarrow NH_2OH + C_6H_5NH_2$	98.0
62	$NH_2NH_2 + CO \rightarrow H_2NC(O)NH_2$	95.7
63	$NH_2NH_2 + CH_3C(O)CH_3 \rightarrow H_2NC(O)NH_2 + CH_3CH_3$	96.7
64	$NH_2NH_2 + CH_3C(O)CH_3 \rightarrow CH_3C(O)NH_2 + CH_3NH_2$	96.0
65	$NH_2NH_2 + CH_3C(O)CH_2CH_3 \rightarrow CH_3C(O)NH_2 + CH_3NHCH_3$	98.0
66	$NH_2NH_2 + 2\ CO \rightarrow H_2NC(O)C(O)NH_2$	98.6
67	$NH_2NH_2 + HC(O)C(O)H \rightarrow H_2NC(O)C(O)NH_2 + H_2$	98.9
68	$NH_2NH_2 + HC(O)H \rightarrow HC(O)NH_2 + NH_3$	94.8
69	$NH_2NH_2 + HC(O)C(O)H \rightarrow 2\ HC(O)NH_2$	96.5
70	$NH_2NH_2 + CH_3C(O)H \rightarrow CH_3C(O)NH_2 + NH_3$	93.5
71	$NH_2NH_2 + CH_3C(O)OH \rightarrow CH_3C(O)NH_2 + NH_2OH$	97.7
72	$NH_2NH_2 + HOC(O)C(O)OH \rightarrow 2\ NH_2OH + 2\ CO$	99.2
73	$NH_2NH_2 + HOC(O)CH_2CH_2C(O)OH \rightarrow 2\ H_2NCH_2C(O)OH$ (Gly)	96.7
74	$NH_2NH_2 + CH_3C(O)OCH_2CH_3 \rightarrow H_2NCH_2CH_2C(O)OH$ (β-Ala) $+ CH_3NH_2$	99.3
75	$NH_2NH_2 + CH_3CN \rightarrow NH_2CN + CH_3NH_2$	97.5
	average of 20 reactions (56-75) with species not from ATcT	**97.3**
	average of all 75 reactions	**97.0**

methylhydrazine: CH_3NHNH_2 (1)

atomization reaction 95.4

reactions with radicals from ATcT

1	$CH_3NHNH_2 + {\bullet}CH_3 \rightarrow {\bullet}NH_2 + CH_3NHCH_3$	93.5
2	$CH_3NHNH_2 + {\bullet}H \rightarrow {\bullet}NH_2 + CH_3NH_2$	94.4
3	$CH_3NHNH_2 + {\bullet}H \rightarrow {\bullet}CH_2NH_2 + NH_3$	91.3

4	$CH_3NHNH_2 + \bullet OH \rightarrow \bullet CH_2NH_2 + NH_2OH$	90.9
5	$CH_3NHNH_2 + \bullet H \rightarrow \bullet NHCH_3 + NH_3$	93.1
6	$CH_3NHNH_2 + \bullet OH \rightarrow \bullet NHCH_3 + NH_2OH$	92.7
7	$CH_3NHNH_2 + \bullet CH_3 \rightarrow \bullet NHNH_2 + CH_3CH_3$	91.9
8	$CH_3NHNH_2 + \bullet OH \rightarrow \bullet NHNH_2 + CH_3OH$	93.5
	average of 8 reactions (1-8) with radicals	**92.7**
reactions with NH_2NH_2		
9	$CH_3NHNH_2 + H_2O \rightarrow NH_2NH_2 + CH_3OH$	92.8
10	$CH_3NHNH_2 + H_2O_2 \rightarrow NH_2NH_2 + CH_3OOH$	92.9
11	$CH_3NHNH_2 + NH3 \rightarrow NH_2NH_2 + CH_3NH_2$	92.3
12	$CH_3NHNH_2 + HCN \rightarrow NH_2NH_2 + CH_3CN$	90.8
13	$CH_3NHNH_2 + CH_4 \rightarrow NH_2NH_2 + CH_3CH_3$	90.1
14	$CH_3NHNH_2 + CH_3CH_3 \rightarrow NH_2NH_2 + CH_3CH_2CH_3$	90.0
15	$CH_3NHNH_2 + H_2C{=}CH_2 \rightarrow NH_2NH_2 + CH_3CH{=}CH_2$	90.1
16	$CH_3NHNH_2 + HC{\equiv}CH \rightarrow NH_2NH_2 + CH_3C{\equiv}CH$	91.1
17	$CH_3NHNH_2 + C_6H_6 \rightarrow NH_2NH_2 + C_6H_5CH_3$	91.2
18	$CH_3NHNH_2 + C_6H_5CH_3 \rightarrow NH_2NH_2 + C_6H_5CH_2CH_3$	92.1
19	$CH_3NHNH_2 + CH_3OH \rightarrow NH_2NH_2 + CH_3OCH_3$	91.3
20	$CH_3NHNH_2 + CH_3OH \rightarrow NH_2NH_2 + CH_3CH_2OH$	88.9
21	$CH_3NHNH_2 + HC(O)H \rightarrow NH_2NH_2 + CH_3C(O)H$	88.6
22	$CH_3NHNH_2 + HC(O)OH \rightarrow NH_2NH_2 + CH_3C(O)OH$	87.7
23	$CH_3NHNH_2 + CH_3C(O)H \rightarrow NH_2NH_2 + CH_3C(O)CH_3$	89.8
	average of 15 reactions (9-23) with NH_2NH_2	**90.6**
reactions without NH_2NH_2		
24	$CH_3NHNH_2 + CH_4 \rightarrow 2\ CH_3NH_2$	92.9
25	$CH_3NHNH_2 + CH_4 \rightarrow CH_3NHCH_3 + NH_3$	92.5
26	$CH_3HNNH_2 \rightarrow CH_4 + NH{=}NH$	93.5
27	$CH_3NHNH_2 + CH_3CH_3 \rightarrow CH_3NH_2 + CH_3NHCH_3$	94.7
28	$CH_3NHNH_2 + CH_3CH_2CH_3 \rightarrow H_2NCH_2CH_2NH_2 + CH_3CH_3$	93.6
29	$CH_3NHNH_2 + H_2C{=}CH_2 \rightarrow HN{=}NH + CH_3CH_2CH_3$	94.4
30	$CH_3NHNH_2 + 2\ C_6H_6 \rightarrow 2\ C_6H_5NH_2 + CH_4$	95.7
31	$CH_3NHNH_2 + C_6H_5CH_3 \rightarrow C_6H_5NH_2 + CH_3NHCH_3$	95.0
32	$CH_3NHNH_2 + H_2O \rightarrow NH_2OH + CH_3NH_2$	94.0
33	$CH_3NHNH_2 + CH_3OH \rightarrow NH_2OH + CH_3NHCH_3$	93.0
34	$CH_3NHNH_2 + CH_3CH_2OH \rightarrow NH_2OH + N(CH_3)_3$	96.1
35	$CH_3NHNH_2 + HOCH_2CH_2OH \rightarrow H_2NCH_2CH_2NH_2 + CH_2(OH)_2$	92.6
36	$CH_3HNNH_2 + C_6H_5CH_2OH \rightarrow C_8H_{11}N$ (2,4-dimethylaniline) $+ NH_2OH$	94.1
37	$CH_3NHNH_2 + HC(O)H \rightarrow HC(O)NH_2 + CH_3NH_2$	91.5
38	$CH_3NHNH_2 + CH_3C(O)H \rightarrow CH_3C(O)NH_2 + CH_3NH_2$	90.2
39	$CH_3NHNH_2 + CH_3C(O)CH_3 \rightarrow H_2NC(O)NH_2 + CH_3CH_2CH_3$	91.2
40	$CH_3NHNH_2 + HC(O)C(O)H \rightarrow H_2NC(O)C(O)NH_2 + CH_4$	92.7
41	$CH_3NHNH_2 + HC(O)OH \rightarrow CH_3C(O)NH_2 + NH_2OH$	89.9
42	$CH_3NHNH_2 + HOC(O)CH_2C(O)OH \rightarrow 2\ H_2NCH_2C(O)OH$ (Gly)	96.0
43	$CH_3NHNH_2 + CH_3CN \rightarrow NH_2CN + CH_3NHCH_3$	93.8
	average of 20 reactions (24-43) without NH_2NH_2	**93.4**

1,1-dimethylhydrazine: $(CH_3)_2NNH_2$ (2)

atomization reaction		83.3
reactions with NH_2NH_2		
1	$(CH_3)_2NNH_2 + H_2O \rightarrow NH_2NH_2 + CH_3OCH_3$	81.1
2	$(CH_3)_2NNH_2 + NH_3 \rightarrow NH_2NH_2 + CH_3NHCH_3$	81.2
3	$(CH_3)_2NNH_2 + CH_4 \rightarrow NH_2NH_2 + CH_3CH_2CH_3$	77.2

4	$(CH_3)_2NNH_2 + CH_3CH_3 \rightarrow NH_2NH_2 + (CH_3)_2CHCH_3$	76.5
5	$(CH_3)_2NNH_2 + H_2C{=}CH_2 \rightarrow NH_2NH_2 + \textit{trans}\text{-}CH_3CH{=}CHCH_3$	76.8
6	$(CH_3)_2NNH_2 + C_6H_6 \rightarrow NH_2NH_2 + C_6H_5CH_2CH_3$	80.4
7	$(CH_3)_2NNH_2 + CH_3OH \rightarrow NH_2NH_2 + CH_3CH(OH)CH_3$	77.4
8	$(CH_3)_2NNH_2 + HC(O)H \rightarrow NH_2NH_2 + CH_3C(O)CH_3$	75.5
9	$(CH_3)_2NNH_2 + CH_3NH_2 \rightarrow NH_2NH_2 + (CH_3)_3N$	80.9
10	$(CH_3)_2NNH_2 + C_6H_5NH_2 \rightarrow C_6H_5N(CH_3)_2 + NH_2NH_2$	79.5
	average of 10 reactions (1-10) with NH2NH2	**78.6**
reactions with CH_3NHNH_2		
11	$(CH_3)_2NNH_2 + H_2O \rightarrow CH_3NHNH_2 + CH_3OH$	84.4
12	$(CH_3)_2NNH_2 + H_2O_2 \rightarrow CH_3NHNH_2 + CH_3OOH$	84.5
13	$(CH_3)_2NNH_2 + NH_3 \rightarrow CH_3NHNH_2 + CH_3NH_2$	83.9
14	$(CH_3)_2NNH_2 + HCN \rightarrow CH_3NHNH_2 + CH_3CN$	82.4
15	$(CH_3)_2NNH_2 + CH_3CH_3 \rightarrow CH_3NHNH_2 + CH_3CH_2CH_3$	81.6
16	$(CH_3)_2NNH_2 + CH_3CH_2CH_3 \rightarrow CH_3NHNH_2 + (CH_3)_2CHCH_3$	81.0
17	$(CH_3)_2NNH_2 + H_2C{=}CH_2 \rightarrow CH_3NHNH_2 + CH_3CH{=}CH_2$	81.7
18	$(CH_3)_2NNH_2 + HC{\equiv}CH \rightarrow CH_3NHNH_2 + CH_3C{\equiv}CH$	82.7
19	$(CH_3)_2NNH_2 + C_6H_6 \rightarrow CH_3NHNH_2 + C_6H_5CH_3$	82.8
20	$(CH_3)_2NNH_2 + C_6H_5CH_3 \rightarrow CH_3NHNH_2 + C_6H_5CH_2CH_3$	83.7
21	$(CH_3)_2NNH_2 + CH_3OH \rightarrow CH_3NHNH_2 + CH_3OCH_3$	82.9
22	$(CH_3)_2NNH_2 + CH_3OH \rightarrow CH_3NHNH_2 + CH_3CH_2OH$	80.5
23	$(CH_3)_2NNH_2 + HC(O)H \rightarrow CH_3NHNH_2 + CH_3C(O)H$	80.2
24	$(CH_3)_2NNH_2 + CH_3C(O)H \rightarrow CH_3NHNH_2 + CH_3C(O)CH_3$	81.4
25	$(CH_3)_2NNH_2 + CH_3NH_2 \rightarrow CH_3NHNH_2 + (CH_3)_2NH$	83.4
	average of 15 reactions (11-25) with CH_3NHNH_2	**82.5**
reactions with different species		
26	$(CH_3)_2NNH_2 + 2\ CH_4 \rightarrow 2\ CH_3NH_2 + CH_3CH_3$	80.1
27	$(CH_3)_2NNH_2 + CH_3CH_3 \rightarrow 2\ CH_3NHCH_3$	83.6
28	$(CH_3)_2NNH_2 \rightarrow H_2NCH_2CH_2NH_2$	80.7
29	$(CH_3)_2NNH_2 + H_2C{=}CH_2 \rightarrow HN{=}NH + (CH_3)_2CHCH_3$	80.9
30	$(CH_3)_2NNH_2 + 2\ C_6H_6 \rightarrow 2\ C_6H_5NH_2 + CH_3CH_3$	82.8
31	$(CH_3)_2NNH_2 + C_6H_6 \rightarrow C_6H_5NH_2 + CH_3NHCH_3$	83.2
32	$(CH_3)_2NNH_2 + H_2O \rightarrow NH_2OH + CH_3NHCH_3$	82.9
33	$(CH_3)_2NNH_2 + CH_3OH \rightarrow (CH_3)_3N + NH_2OH$	82.1
34	$(CH_3)_2NNH_2 + C_6H_5CH_2OH \rightarrow 1,4\text{-}CH_3C_6H_4N(CH_3)_2 + NH_2OH$	80.4
35	$(CH_3)_2NNH_2 + HC(O)H \rightarrow HC(O)NH_2 + CH_3NHCH_3$	80.4
36	$(CH_3)_2NNH_2 + HC(O)OH \rightarrow H_2NCH_2C(O)OH\ (Gly) + CH_3NH_2$	81.7
37	$(CH_3)_2NNH_2 + HC(O)OH \rightarrow CH_3CH(NH_2)C(O)OH\ (Ala) + NH_3$	80.9
38	$(CH_3)_2NNH_2 + CH_3C(O)OH \rightarrow H_2NCH_2C(O)OH\ (Gly) + CH_3NHCH_3$	85.8
39	$(CH_3)_2NNH_2 + CH_3C(O)OH \rightarrow CH_3CH(NH_2)C(O)OH\ (Ala) + CH_3NH_2$	85.4
40	$(CH_3)_2NNH_2 + HCN \rightarrow NH_2CN + CH_3NHCH_3$	81.7
	average of 15 reactions (26-40) with different species	**82.2**
	average of 30 reactions (11-40) with CH_3NHNH_2 and different species	**82.3**

1,2-dimethylhydrazine: $CH_3NHNHCH_3$ (3)

atomization reaction		95.4
reactions with NH_2NH_2		
1	$CH_3NHNHCH_3 + H_2O \rightarrow NH_2NH_2 + CH_3OCH_3$	93.3
2	$CH_3NHNHCH_3 + NH_3 \rightarrow NH_2NH_2 + CH_3NHCH_3$	93.4
3	$CH_3NHNHCH_3 + CH_4 \rightarrow NH_2NH_2 + CH_3CH_2CH_3$	89.4
4	$CH_3NHNHCH_3 + CH_3CH_3 \rightarrow NH_2NH_2 + (CH_3)_2CHCH_3$	88.7

5	$CH_3NHNHCH_3 + H_2C{=}CH_2 \rightarrow NH_2NH_2 + \textit{trans}\text{-}CH_3CH_2CH{=}CH_2$	88.9
6	$CH_3NHNHCH_3 + C_6H_6 \rightarrow NH_2NH_2 + C_6H_5CH_2CH_3$	92.5
7	$CH_3NHNHCH_3 + CH_3OH \rightarrow NH_2NH_2 + CH_3CH(OH)CH_3$	89.5
8	$CH_3NHNHCH_3 + HC(O)H \rightarrow NH_2NH_2 + CH_3C(O)CH_3$	87.7
9	$CH_3NHNHCH_3 + CH_3NH_2 \rightarrow NH_2NH_2 + (CH_3)_3N$	93.1
10	$CH_3NHNHCH_3 + C_6H_5NH_2 \rightarrow NH_2NH_2 + C_6H_5N(CH_3)_2$	91.7
	average of 10 reactions (1-10) with NH_2NH_2	**90.8**
	reactions with CH_3NHNH_2	
11	$CH_3NHNHCH_3 + H_2O \rightarrow CH_3NHNH_2 + CH_3OH$	96.5
12	$CH_3NHNHCH_3 + H_2O_2 \rightarrow CH_3NHNH_2 + CH_3OOH$	96.7
13	$CH_3NHNHCH_3 + NH_3 \rightarrow CH_3NHNH_2 + CH_3NH_2$	96.0
14	$CH_3NHNHCH_3 + HCN \rightarrow CH_3NHNH_2 + CH_3CN$	94.6
15	$CH_3NHNHCH_3 + CH_3CH_3 \rightarrow CH_3NHNH_2 + CH_3CH_2CH_3$	93.8
16	$CH_3NHNHCH_3 + CH_3CH_2CH_3 \rightarrow CH_3NHNH_2 + (CH_3)_2CHCH_3$	93.2
17	$CH_3NHNHCH_3 + H_2C{=}CH_2 \rightarrow CH_3NHNH_2 + CH_3CH{=}CH_2$	93.8
18	$CH_3NHNHCH_3 + HC{\equiv}CH \rightarrow CH_3NHNH_2 + CH_3C{\equiv}CH$	94.9
19	$CH_3NHNHCH_3 + C_6H_6 \rightarrow CH_3NHNH_2 + C_6H_5CH_3$	94.9
20	$CH_3NHNHCH_3 + C_6H_5CH_3 \rightarrow CH_3NHNH_2 + C_6H_5CH_2CH_3$	95.9
21	$CH_3NHNHCH_3 + CH_3OH \rightarrow CH_3NHNH_2 + CH_3OCH_3$	95.0
22	$CH_3NHNHCH_3 + CH_3OH \rightarrow CH_3NHNH_2 + CH_3CH_2OH$	92.7
23	$CH_3NHNHCH_3 + HC(O)H \rightarrow CH_3NHNH_2 + CH_3C(O)H$	92.4
24	$CH_3NHNHCH_3 + CH_3C(O)H \rightarrow CH_3NHNH_2 + CH_3C(O)CH_3$	93.6
25	$CH_3NHNHCH_3 + CH_3NH_2 \rightarrow CH_3NHNH_2 + (CH_3)_2NH$	95.6
	average of 15 reactions (11-25) with CH_3NHNH_2	**94.6**
	reaction with $(CH_3)_2NNH_2$	
26	$CH_3NHNHCH_3 \rightarrow (CH_3)_2NNH_2$	**95.5**
	reactions with different species	
27	$CH_3NHNHCH_3 + 2\ CH_4 \rightarrow 2\ CH_3NH_2 + CH_3CH_3$	92.3
28	$CH_3NHNHCH_3 + CH_3CH_3 \rightarrow 2\ CH_3NHCH_3$	95.8
29	$CH_3NHNHCH_3 \rightarrow H_2NCH_2CH_2NH_2$	92.9
30	$CH_3NHNHCH_3 + H_2C{=}CH_2 \rightarrow HN{=}NH + (CH_3)_2CHCH3$	93.1
31	$CH_3NHNHCH_3 + 2\ C_6H_6 \rightarrow 2\ C_6H_5NH_2 + CH_3CH_3$	95.0
32	$CH_3NHNHCH_3 + C_6H_6 \rightarrow C_6H_5NH_2 + CH_3NHCH_3$	95.4
33	$CH_3NHNHCH_3 + H_2O \rightarrow NH_2OH + CH_3NHCH_3$	95.1
34	$CH_3NHNHCH_3 + CH_3OH \rightarrow (CH_3)_3N + NH_2OH$	94.3
35	$CH_3NHNHCH_3 + C_6H_5CH_2OH \rightarrow 1,4\text{-}CH_3C_6H_4N(CH_3)_2 + NH_2OH$	92.5
36	$CH_3NHNHCH_3 + HC(O)H \rightarrow HC(O)NH_2 + CH_3NHCH_3$	92.6
37	$CH_3NHNHCH_3 + HC(O)OH \rightarrow H_2NCH_2C(O)OH\ (Gly) + CH_3NH_2$	93.9
38	$CH_3NHNHCH_3 + HC(O)OH \rightarrow CH_3CH(NH_2)C(O)OH\ (Ala) + NH_3$	93.1
39	$CH_3NHNHCH_3 + CH_3C(O)OH \rightarrow H_2NCH_2C(O)OH\ (Gly) + CH_3NHCH_3$	98.0
40	$CH_3NHNHCH_3 + CH_3C(O)OH \rightarrow CH_3CH(NH_2)C(O)OH\ (Ala) + CH_3NH_2$	97.6
41	$CH_3NHNHCH_3 + HCN \rightarrow NH_2CN + CH_3NHCH_3$	93.8
	average of 15 reactions (27-41) with different molecules	**94.4**
	average of 31 reactions (11-41) with CH_3NHNH_2, $(CH_3)_2NNH_2$, and different species	**94.8**

ethylhydrazine: $CH_3CH_2NHNH_2$ (4)

	atomization reaction	67.1
	reactions with different species	
1	$CH_3CH_2NHNH_2 \rightarrow (CH_3)_2NNH_2$	67.1
2	$CH_3CH_2NHNH_2 + CH_3CH_3 \rightarrow CH_3NHNH_2 + CH_3CH_2CH_3$	65.5

3	$CH_3CH_2NHNH_2 + 2\ CH_4 \rightarrow 2\ CH_3NH_2 + CH_3CH_3$	63.9
4	$CH_3CH_2NHNH_2 + CH_3CH_3 \rightarrow 2\ CH_3NHCH_3$	67.5
5	$CH_3CH_2NHNH_2 + H_2C{=}CH_2 \rightarrow HN{=}NH + (CH_3)_2CHCH_3$	64.8
6	$CH_3CH_2NHNH_2 + CH_3OH \rightarrow (CH_3)_3N + NH_2OH$	65.9
7	$CH_3CH_2NHNH_2 + H_2O \rightarrow NH_2OH + CH_3NHCH_3$	66.7
8	$CH_3CH_2NHNH_2 + HCN \rightarrow NH_2CN + CH_3NHCH_3$	65.5
9	$CH_3CH_2NHNH_2 \rightarrow H_2NCH_2CH_2NH_2$	64.5
10	$CH_3CH_2NHNH_2 + HC(O)OH \rightarrow H_2NCH_2C(O)OH$ (Gly) $+ CH_3NH_2$	65.5
	average of 10 reactions	**65.7**

trimethylhydrazine: $(CH_3)_2NNHCH_3$ (5)

atomization reaction		82.4
reactions with CH_3NHNH_2		
1	$(CH_3)_2NNHCH_3 + H_2O \rightarrow CH_3NHNH_2 + CH_3OCH_3$	84.1
2	$(CH_3)_2NNHCH_3 + NH_3 \rightarrow CH_3NHNH_2 + CH_3NHCH_3$	84.2
3	$(CH_3)_2NNHCH_3 + CH_4 \rightarrow CH_3NHNH_2 + CH_3CH_2CH_3$	80.2
4	$(CH_3)_2NNHCH_3 + CH_3CH_3 \rightarrow CH_3NHNH_2 + (CH_3)_2CHCH_3$	79.5
5	$(CH_3)_2NNHCH_3 + CH_3CH_2CH_3 \rightarrow CH_3NHNH_2 + (CH_3)_2CHCH_2CH_3$	80.5
6	$(CH_3)_2NNHCH_3 + H_2C{=}CH_2 \rightarrow CH_3NHNH_2 + CH_3CH{=}CHCH_3$	79.7
7	$(CH_3)_2NNHCH_3 + HC{\equiv}CH \rightarrow CH_3NHNH_2 + CH_3C{\equiv}CCH_3$	79.1
8	$(CH_3)_2NNHCH_3 + C_6H_6 \rightarrow CH_3NHNH_2 + C_6H_5CH_2CH_3$	83.3
9	$(CH_3)_2NNHCH_3 + C_6H_5CH_3 \rightarrow CH_3NHNH_2 + C_9H_{12}$ (1,3,5-trimethylbenzene)	81.3
10	$(CH_3)_2NNHCH_3 + CH_3OH \rightarrow CH_3NHNH_2 + CH_3CH(OH)CH_3$	80.3
11	$(CH_3)_2NNHCH_3 + CH_3NH_2 \rightarrow CH_3NHNH_2 + (CH_3)_3N$	83.8
12	$(CH_3)_2NNHCH_3 + C_6H_5NH_2 \rightarrow CH_3NHNH_2 + C_6H_5N(CH_3)_2$	82.5
	average of 12 reactions (1-12) with CH_3NHNH_2	**81.5**
reactions with $(CH_3)_2NNH_2$		
13	$(CH_3)_2NNHCH_3 + H_2O \rightarrow (CH_3)_2NNH_2 + CH_3OH$	84.5
14	$(CH_3)_2NNHCH_3 + H_2O_2 \rightarrow (CH_3)_2NNH_2 + CH_3OOH$	84.7
15	$(CH_3)_2NNHCH_3 + NH_3 \rightarrow (CH_3)_2NNH_2 + CH_3NH_2$	84.0
16	$(CH_3)_2NNHCH_3 + CH_4 \rightarrow (CH_3)_2NNH_2 + CH_3CH_3$	81.8
17	$(CH_3)_2NNHCH_3 + CH_3CH_3 \rightarrow (CH_3)_2NNH_2 + CH_3CH_2CH_3$	81.8
18	$(CH_3)_2NNHCH_3 + CH_3CH_2CH_3 \rightarrow (CH_3)_2NNH_2 + (CH_3)_2CHCH_3$	81.1
19	$(CH_3)_2NNHCH_3 + H_2C{=}CH_2 \rightarrow (CH_3)_2NNH_2 + CH_3CH{=}CH_2$	81.8
20	$(CH_3)_2NNHCH_3 + CH_3CH{=}CH_2 \rightarrow (CH_3)_2NNH_2 + CH_3CH{=}CHCH_3$	81.4
21	$(CH_3)_2NNHCH_3 + HC{\equiv}CH \rightarrow (CH_3)_2NNH_2 + CH_3C{\equiv}CH$	82.9
22	$(CH_3)_2NNHCH_3 + CH_3C{\equiv}CH \rightarrow (CH_3)_2NNH_2 + CH_3C{\equiv}CCH_3$	79.6
23	$(CH_3)_2NNHCH_3 + C_6H_6 \rightarrow (CH_3)_2NNH_2 + C_6H_5CH_3$	82.9
24	$(CH_3)_2NNHCH_3 + C_6H_5CH_3 \rightarrow (CH_3)_2NNH_2 + C_6H_5CH_2CH_3$	83.8
25	$(CH_3)_2NNHCH_3 + CH_3OH \rightarrow (CH_3)_2NNH_2 + CH_3CH_2OH$	80.7
26	$(CH_3)_2NNHCH_3 + CH_3CH_2OH \rightarrow (CH_3)_2NNH_2 + CH_3CH(OH)CH_3$	83.1
27	$(CH_3)_2NNHCH_3 + HC(O)H \rightarrow (CH_3)_2NNH_2 + CH_3C(O)H$	80.4
28	$(CH_3)_2NNHCH_3 + CH_3C(O)H \rightarrow (CH_3)_2NNH_2 + CH_3C(O)CH_3$	81.6
29	$(CH_3)_2NNHCH_3 + CH_3C(O)CH_3 \rightarrow (CH_3)_2NNH_2 + CH_3C(O)CH_2CH_3$	81.6
30	$(CH_3)_2NNHCH_3 + HC(O)OH \rightarrow (CH_3)_2NNH_2 + CH_3C(O)OH$	79.5
31	$(CH_3)_2NNHCH_3 + CH_3NH_2 \rightarrow (CH_3)_2NNH_2 + CH_3NHCH_3$	83.6
32	$(CH_3)_2NNHCH_3 + CH_3NHCH_3 \rightarrow (CH_3)_2NNH_2 + (CH_3)_3N$	83.7
	average of 20 reactions (13-32) with $(CH_3)_2NNH_2$	**82.2**
reactions with different species		
33	$(CH_3)_2NNHCH_3 + CH_4 \rightarrow (CH_3)_3N + CH_3NH_2$	82.3
34	$(CH_3)_2NNHCH_3 + CH_4 \rightarrow 2\ CH_3NHCH_3$	82.2
35	$(CH_3)_2NNHCH_3 + CH_4 \rightarrow H_2NCH_2CH_2NH_2 + CH_3CH_3$	79.2

36	$(CH_3)_2NNHCH_3 + CH_3CH_3 \rightarrow CH_3NHCH_3 + (CH_3)_3N$	84.0
37	$(CH_3)_2NNHCH_3 + CH_3CH_2CH_3 \rightarrow 2\ (CH_3)_3N$	85.9
38	$(CH_3)_2NNHCH_3 \rightarrow HN{=}NH + CH_3CH_2CH_3$	79.2
39	$(CH_3)_2NNHCH_3 + H_2C{=}CH_2 \rightarrow HN{=}NH + (CH_3)_2CHCH_2CH_3$	80.5
40	$(CH_3)_2NNHCH_3 + 2\ C_6H_6 \rightarrow 2\ C_6H_5NH_2 + CH_3CH_2CH_3$	81.3
41	$(CH_3)_2NNHCH_3 + C_6H_6 \rightarrow C_6H_5NH_2 + (CH_3)_3N$	83.6
42	$(CH_3)_2NNHCH_3 + C_6H_5CH_3 \rightarrow C_6H_5N(CH_3)_2 + CH_3NHCH_3$	82.9
43	$(CH_3)_2NNHCH_3 + C_6H_5CH_3 \rightarrow C_6H_5NHCH_2CH_3 + CH_3NHCH_3$	84.0
44	$(CH_3)_2NNHCH_3 + H_2O \rightarrow NH_2OH + (CH_3)_3N$	83.3
45	$(CH_3)_2NNHCH_3 + HC(O)OH \rightarrow H_2NCH_2C(O)OH$ (Gly) $+ CH_3NHCH_3$	82.0
46	$(CH_3)_2NNHCH_3 + HC(O)OH \rightarrow CH_3CH(NH_2)C(O)OH$ (Ala) $+ CH_3NH_2$	81.6
47	$(CH_3)_2NNHCH_3 + CH_3C(O)OH \rightarrow CH_3CH(NH_2)C(O)OH$ (Ala) $+ CH_3NHCH_3$	85.7
	average of 15 reactions (33-47) with different species	**82.5**
	average of all 47 reactions	**82.1**

isopropylhydrazine: $(CH_3)_2CHNHNH_2$ (6)

atomization reaction 32.2

reactions with different species

1	$(CH_3)_2CHNHNH_2 + NH_3 \rightarrow CH_3NHNH_2 + CH_3NHCH_3$	33.9
2	$(CH_3)_2CHNHNH_2 + CH_4 \rightarrow CH_3NHNH_2 + CH_3CH_2CH_3$	30.0
3	$(CH_3)_2CHNHNH_2 + CH_3CH_3 \rightarrow CH_3NHNH_2 + (CH_3)_2CHCH_3$	29.3
4	$(CH_3)_2CHNHNH_2 + CH_3OH \rightarrow CH_3NHNH_2 + CH_3CH(OH)CH_3$	30.1
5	$(CH_3)_2CHNHNH_2 + H_2C{=}CH_2 \rightarrow CH_3NHNH_2 + CH_3CH{=}CHCH_3$	29.5
6	$(CH_3)_2CHNHNH_2 + CH_3CH_3 \rightarrow (CH_3)_2NNH_2 + CH_3CH_2CH_3$	31.6
7	$(CH_3)_2CHNHNH_2 + H_2C{=}CH_2 \rightarrow (CH_3)_2NNH_2 + CH_3CH{=}CH_2$	31.6
8	$(CH_3)_2CHNHNH_2 + CH_3OH \rightarrow (CH_3)_2NNH_2 + CH_3CH_2OH$	30.4
9	$(CH_3)_2CHNHNH_2 + CH_3NH_2 \rightarrow (CH_3)_2NNH_2 + CH_3NHCH_3$	33.4
10	$(CH_3)_2CHNHNH_2 + HC(O)H \rightarrow (CH_3)_2NNH_2 + CH_3C(O)H$	30.1
11	$(CH_3)_2CHNHNH_2 + CH_4 \rightarrow 2\ CH_3NHCH_3$	31.9
12	$(CH_3)_2CHNHNH_2 + CH_3CH_3 \rightarrow CH_3NHCH_3 + (CH_3)_3N$	33.8
13	$(CH_3)_2CHNHNH_2 + CH_4 \rightarrow H_2NCH_2CH_2NH_2 + CH_3CH_3$	29.0
14	$(CH_3)_2CHNHNH_2 + C_6H_6 \rightarrow C_6H_5NH_2 + (CH_3)_3N$	33.4
15	$(CH_3)_2CHNHNH_2 + HC(O)OH \rightarrow H_2NCH_2C(O)OH$ (Gly) $+ CH_3NHCH_3$	31.8
	average of 15 reactions	**31.3**

tetramethylhydrazine: $(CH_3)_2NN(CH_3)_2$ (7)

atomization reaction 81.2

reactions with CH_3NHNH_2

1	$(CH_3)_2NN(CH_3)_2 + H_2O \rightarrow CH_3NHNH_2 + CH_3CH(OH)CH_3$	81.2
2	$(CH_3)_2NN(CH_3)_2 + NH_3 \rightarrow CH_3NHNH_2 + (CH_3)_3N$	84.2
3	$(CH_3)_2NN(CH_3)_2 + CH_3NH_2 \rightarrow CH_3NHNH_2 + CH_3CH_2NHCH_2CH_3$	81.9
4	$(CH_3)_2NN(CH_3)_2 + CH_4 \rightarrow CH_3NHNH_2 + (CH_3)_2CHCH_3$	77.7
5	$(CH_3)_2NN(CH_3)_2 + CH_3CH_3 \rightarrow CH_3NHNH_2 + (CH_3)_2CHCH_2CH_3$	78.6
6	$(CH_3)_2NN(CH_3)_2 + CH_3CH_2CH_3 \rightarrow CH_3NHNH_2 + (CH_3)_2CHCH(CH_3)_2$	78.7
7	$(CH_3)_2NN(CH_3)_2 + C_6H_6 \rightarrow CH_3NHNH_2 + C_6H_5CH(CH_3)_2$	83.5
8	$(CH_3)_2NN(CH_3)_2 + C_6H_6 \rightarrow CH_3NHNH_2 + C_9H_{12}$ (1,3,5-trimethylbenzene)	80.6
9	$(CH_3)_2NN(CH_3)_2 + C_6H_5CH_3 \rightarrow CH_3NHNH_2 + C_6H_5C(CH_3)_3$	82.5
10	$(CH_3)_2NN(CH_3)_2 + CH_3OH \rightarrow CH_3NHNH_2 + CH_3CH_2CH_2CH_2OH$	78.6
11	$(CH_3)_2NN(CH_3)_2 + CH_3OH \rightarrow CH_3NHNH_2 + CH_3CH_2OCH_2CH_3$	79.8
12	$(CH_3)_2NN(CH_3)_2 + HC(O)H \rightarrow CH_3NHNH_2 + CH_3C(O)CH_2CH_3$	76.4
13	$(CH_3)_2NN(CH_3)_2 + HC(O)OH \rightarrow CH_3NHNH_2 + (CH_3)_2CHC(O)OH$	80.0

	average of 13 reactions (1-13) with CH_3NHNH_2	**80.3**
reactions with $(CH_3)_2NNH_2$		
14	$(CH_3)_2NN(CH_3)_2 + H_2O \rightarrow (CH_3)_2NNH_2 + CH_3CH_2OH$	81.5
15	$(CH_3)_2NN(CH_3)_2 + H_2O \rightarrow (CH_3)_2NNH_2 + CH_3OCH_3$	83.9
16	$(CH_3)_2NN(CH_3)_2 + NH_3 \rightarrow (CH_3)_2NNH_2 + CH_3NHCH_3$	84.0
17	$(CH_3)_2NN(CH_3)_2 + CH_4 \rightarrow (CH_3)_2NNH_2 + CH_3CH_2CH_3$	80.0
18	$(CH_3)_2NN(CH_3)_2 + CH_3CH_3 \rightarrow (CH_3)_2NNH_2 + (CH_3)_2CHCH_3$	79.3
19	$(CH_3)_2NN(CH_3)_2 + CH_3CH_2CH_3 \rightarrow (CH_3)_2NNH_2 + (CH_3)_2CHCH_2CH_3$	80.3
20	$(CH_3)_2NN(CH_3)_2 + H_2C{=}CH_2 \rightarrow (CH_3)_2NNH_2 + CH_3CH{=}CHCH_3$	79.5
21	$(CH_3)_2NN(CH_3)_2 + HC{\equiv}CH \rightarrow (CH_3)_2NNH_2 + CH_3C{\equiv}CCH_3$	78.9
22	$(CH_3)_2NN(CH_3)_2 + C_6H_6 \rightarrow (CH_3)_2NNH_2 + C_6H_5CH_2CH_3$	83.1
23	$(CH_3)_2NN(CH_3)_2 + C_6H_5CH_3 \rightarrow (CH_3)_2NNH_2 + C_6H_5CH(CH_3)_2$	84.1
24	$(CH_3)_2NN(CH_3)_2 + CH_3OH \rightarrow (CH_3)_2NNH_2 + CH_3CH(OH)CH_3$	80.1
25	$(CH_3)_2NN(CH_3)_2 + CH_3OCH_3 \rightarrow (CH_3)_2NNH_2 + CH_3CH_2OCH_2CH_3$	80.2
26	$(CH_3)_2NN(CH_3)_2 + CH_3CH_2OH \rightarrow (CH_3)_2NNH_2 + CH_3CH_2CH_2CH_2OH$	81.4
27	$(CH_3)_2NN(CH_3)_2 + HC(O)H \rightarrow (CH_3)_2NNH_2 + CH_3C(O)CH_3$	78.3
28	$(CH_3)_2NN(CH_3)_2 + CH_3C(O)H \rightarrow (CH_3)_2NNH_2 + CH_3C(O)CH_2CH_3$	79.5
29	$(CH_3)_2NN(CH_3)_2 + CH_3NH_2 \rightarrow (CH_3)_2NNH_2 + (CH_3)_3N$	83.6
30	$(CH_3)_2NN(CH_3)_2 + CH_3NHCH_3 \rightarrow (CH_3)_2NNH_2 + CH_3CH_2NHCH_2CH_3$	81.7
	average of 17 reactions (14-30) with $(CH_3)_2NNH_2$	**81.1**
reactions with different species		
31	$(CH_3)_2NN(CH_3)_2 + 2\ CH_4 \rightarrow 2\ CH_3NH_2 + (CH_3)_2CHCH_3$	76.1
32	$(CH_3)_2NN(CH_3)_2 + 2\ CH_4 \rightarrow 2\ CH_3NHCH_3 + CH_3CH_3$	80.4
33	$(CH_3)_2NN(CH_3)_2 + CH_4 \rightarrow H_2NCH_2CH_2NH_2 + CH_3CH_2CH_3$	77.4
34	$(CH_3)_2NN(CH_3)_2 + CH_4 \rightarrow CH_3NHCH_3 + (CH_3)_3N$	82.2
35	$(CH_3)_2NN(CH_3)_2 + CH_3CH_3 \rightarrow 2\ (CH_3)_3N$	84.1
36	$(CH_3)_2NN(CH_3)_2 \rightarrow HN{=}NH + (CH_3)2CHCH_3$	76.6
37	$(CH_3)_2NN(CH_3)_2 + H_2C{=}CH_2 \rightarrow HN{=}NH + (CH_3)_2CHCH(CH_3)_2$	78.6
38	$(CH_3)_2NN(CH_3)_2 + 2\ C_6H_6 \rightarrow 2\ C_6H_5NH_2 + (CH_3)_2CHCH_3$	78.8
39	$(CH_3)_2NN(CH_3)_2 + C_6H_6 \rightarrow C_6H_5NH_2 + CH_3CH_2NHCH_2CH_3$	81.7
40	$(CH_3)_2NN(CH_3)_2 + C_6H_5CH_3 \rightarrow C_6H_5N(CH_3)_2 + (CH_3)_3N$	83.0
41	$(CH_3)_2NN(CH_3)_2 + C_6H_5CH_3 \rightarrow C_6H_5NHCH_2CH_3 + (CH_3)_3N$	84.0
42	$(CH_3)_2NN(CH_3)_2 + H_2O \rightarrow NH_2OH + CH_3CH_2NHCH_2CH_3$	81.4
43	$(CH_3)_2NN(CH_3)_2 + HC(O)OH \rightarrow H_2NCH_2C(O)OH\ (Gly) + (CH_3)_3N$	82.0
44	$(CH_3)_2NN(CH_3)_2 + HC(O)OH \rightarrow CH_3CH(NH_2)C(O)OH\ (Ala) + CH_3NHCH_3$	81.6
45	$(CH_3)_2NN(CH_3)_2 + CH_3C(O)OH \rightarrow CH_3CH(NH_2)C(O)OH\ (Ala) + (CH_3)_3N$	85.7
	average of 15 reactions (31-45) with different species	**80.9**
	average of all 45 reactions	**80.8**

tert-butylhydrazine: $(CH_3)_3CNHNH_2$ (8)

atomization reaction		-1.9
reactions with different species		
1	$(CH_3)_3CNHNH_2 + H_2O \rightarrow CH_3NHNH_2 + CH_3CH(OH)CH_3$	-2.0
2	$(CH_3)_3CNHNH_2 + NH_3 \rightarrow CH_3NHNH_2 + (CH_3)_3N$	1.0
3	$(CH_3)_3CNHNH_2 + CH_4 \rightarrow CH_3NHNH_2 + (CH_3)_2CHCH_3$	-5.5
4	$(CH_3)_3CNHNH_2 + CH_3OH \rightarrow CH_3NHNH_2 + CH_3CH_2OCH_2CH_3$	-3.4
5	$(CH_3)_3CNHNH_2 + CH_3NH_2 \rightarrow CH_3NHNH_2 + CH_3CH_2NHCH_2CH_3$	-1.3
6	$(CH_3)_3CNHNH_2 + CH_3CH_3 \rightarrow (CH_3)_2NNH_2 + (CH_3)_2CHCH_3$	-3.9
7	$(CH_3)_3CNHNH_2 + H_2C{=}CH_2 \rightarrow (CH_3)_2NNH_2 + CH_3CH{=}CHCH_3$	-3.7
8	$(CH_3)_3CNHNH_2 + CH_3OH \rightarrow (CH_3)_2NNH_2 + CH_3CH(OH)CH_3$	-3.1
9	$(CH_3)_3CNHNH_2 + CH_3NH_2 \rightarrow (CH_3)_2NNH_2 + (CH_3)_3N$	0.5

10	$(CH_3)_3CNHNH_2 + CH_3OCH_3 = (CH_3)_2NNH_2 + CH_3CH_2OCH_2CH_3$	-2.9
11	$(CH_3)_3CNHNH_2 + 2\ CH_4 = 2\ CH_3NHCH_3 + CH_3CH_3$	-2.8
12	$(CH_3)_3CNHNH_2 + CH_3CH_3 = 2\ (CH_3)_3N$	0.9
13	$(CH_3)_3CNHNH_2 + H_2O = NH_2OH + CH_3CH_2NHCH_2CH_3$	-1.8
14	$(CH_3)_3CNHNH_2 + C_6H_5CH_3 = C_6H_5N(CH_3)_2 + (CH_3)_3N$	-0.2
15	$(CH_3)_3CNHNH_2 + HC(O)OH = CH_3CH(NH_2)C(O)OH$ (Ala) $+ CH_3NHCH_3$	-1.6
	average of 15 reactions	**-2.0**

1-methyl-1-nitrosohydrazine: $H_2NN(CH_3)(NO)$ (9)

atomization reaction		161.5
reactions with different species		
1	$H_2NN(CH_3)(NO) \rightarrow CH_3NO + HN{=}NH$	160.5
2	$H_2NN(CH_3)(NO) \rightarrow HC(O)NH_2 + HN{=}NH$	159.5
3	$H_2NN(CH_3)(NO) + H_2 \rightarrow H_2NNHCH_3 + HNO$	161.3
4	$H_2NN(CH_3)(NO) + 2\ CH_4 \rightarrow H_2NNHCH_3 + HNO + CH_3CH_3$	162.0
5	$H_2NN(CH_3)(NO) + CH_4 \rightarrow H_2NNHCH_3 + CH_3NO$	161.5
6	$H_2NN(CH_3)(NO) + CH_4 \rightarrow H_2NNHCH_3 + HC(O)NH_2$	160.5
7	$H_2NN(CH_3)(NO) + CH_4 \rightarrow H_2NN(CH_3)_2 + HNO$	163.6
8	$H_2NN(CH_3)(NO) + CH_3CH_3 \rightarrow H_2NN(CH_3)_2 + CH_3NO$	163.1
9	$H_2NN(CH_3)(NO) + CH_3CH_3 \rightarrow H_2NN(CH_3)_2 + HC(O)NH_2$	162.1
10	$H_2NN(CH_3)(NO) \rightarrow HN_3 + CH_3OH$	162.9
	average of 10 reactions	**161.7**

ethylenedinitrosohydrazine: $H_2NN(NO)CH_2CH_2N(NO)NH_2$ (10)

atomization reaction		345.0
reactions with different species		
1	$H_2NN(NO)CH_2CH_2N(NO)NH_2 + H_2 \rightarrow 2\ CH_3NO + 2\ HN{=}NH$	341.6
2	$H_2NN(NO)CH_2CH_2N(NO)NH_2 + 2\ CH_4 \rightarrow 2\ CH_3NO + 2\ HN{=}NH + CH_3CH_3$	342.3
3	$H_2NN(NO)CH_2CH_2N(NO)NH_2 + 2\ CH_4 \rightarrow 2\ HC(O)NH_2 + 2\ HN{=}NH + CH_3CH_3$	340.3
4	$H_2NN(NO)CH_2CH_2N(NO)NH_2 + 2\ CH_4 \rightarrow 2\ HC(O)NH_2 + 2\ HN{=}NH + CH_3CH_3$	340.3
5	$H_2NN(NO)CH_2CH_2N(NO)NH_2 \rightarrow 2\ HN_3 + HOCH_2CH_2OH$	346.4
6	$H_2NN(NO)CH_2CH_2N(NO)NH_2 \rightarrow 2\ HN_3 + CH_3OOCH_3$	343.4
7	$H_2NN(NO)CH_2CH_2N(NO)NH_2 + CH_3CH_3 + 2\ H_2 \rightarrow 2\ H_2NNHCH3 + 2\ CH_3NO$	342.9
8	$H_2NN(NO)CH_2CH_2N(NO)NH_2 + 4\ CH_4 \rightarrow 2\ H_2NNHCH_3 + 2\ HC(O)NH_2 + CH_3CH_3$	342.4
9	$H_2NN(NO)CH_2CH_2N(NO)NH_2 + 2\ CH_3CH_3 + H_2 \rightarrow 2\ H_2NN(CH_3)_2 + 2\ CH_3NO$	346.8
10	$H_2NN(NO)CH_2CH_2N(NO)NH_2 + 2\ CH_3CH_3 + H_2 \rightarrow 2\ H_2NN(CH_3)_2 + 2\ HC(O)NH_2$	344.9
11	$H_2NN(NO)CH_2CH_2N(NO)NH_2 + 2\ CH_4 \rightarrow 2\ H_2NN(CH_3)(NO) + CH_3CH_3$	344.7
	average of 11 reactions	**343.3**

phenylhydrazine: $C_6H_5NHNH_2$ (11)

atomization reaction		209.7
reactions with CH_3NHNH_2		
1	$C_6H_5NHNH_2 + CH_3CH_3 \rightarrow CH_3NHNH_2 + C_6H_5CH_3$	208.2
2	$C_6H_5NHNH_2 + CH_3CH_2OH \rightarrow CH_3NHNH_2 + C_6H_5CH_2OH$	210.3
3	$C_6H_5NHNH_2 + CH_3OCH_3 \rightarrow CH_3NHNH_2 + C_6H_5OCH_3$	207.1
4	$C_6H_5NHNH_2 + CH_3NH_2 \rightarrow CH_3NHNH_2 + C_6H_5NH_2$	208.5
5	$C_6H_5NHNH_2 + CH_3CH{=}CH_2 \rightarrow CH_3NHNH_2 + C_6H_5CH{=}CH_2$	208.0
	average of 5 reactions (1-5) with CH_3NHNH_2	**208.4**

reactions with $(CH_3)_2NNH_2$

6	$C_6H_5NHNH_2 + CH_3CH_2CH_3 \rightarrow (CH_3)_2NNH_2 + C_6H_5CH_3$	209.9
7	$C_6H_5NHNH_2 + CH_3CH(OH)CH_3 \rightarrow (CH_3)_2NNH_2 + C_6H_5CH_2OH$	210.7
8	$C_6H_5NHNH_2 + CH_3CH(OH)CH_3 \rightarrow (CH_3)_2NNH_2 + C_6H_5OCH_3$	209.8
9	$C_6H_5NHNH_2 + CH_3NHCH_3 \rightarrow (CH_3)_2NNH_2 + C_6H_5NH_2$	208.3
10	$C_6H_5NHNH_2 + CH_3CH=CHCH_3 \rightarrow (CH_3)_2NNH_2 + C_6H_5CH=CH_2$	210.1

average of 5 reactions (6-10) with $(CH_3)_2NNH_2$ 209.7

reactions with different species

11	$C_6H_5NHNH_2 + CH_3CH_3 \rightarrow C_6H_5NH_2 + CH_3NHCH_3$	208.7
12	$C_6H_5NHNH_2 + CH_3CH_3 \rightarrow C_6H_5NHCH_3 + CH_3NH_2$	205.6
13	$C_6H_5NHNH_2 + CH_3CH_3 \rightarrow C_6H_5N(CH_3)_2 + NH_3$	207.0
14	$C_6H_5NHNH_2 + CH_3CH_2CH_3 \rightarrow H_2NCH_2CH_2NH_2 + C_6H_5CH_3$	207.3
15	$C_6H_5NHNH_2 + CH_3CH_2CH_3 \rightarrow C_6H_5NHCH_2CH_3 + CH_3NH_2$	210.3
16	$C_6H_5NHNH_2 \rightarrow C_6H_6 + NH=NH$	206.1
17	$C_6H_5NHNH_2 + H_2O \rightarrow C_6H_5NH_2 + NH_2OH$	207.9
18	$C_6H_5NHNH_2 + 2\ CH_3CH_3 \rightarrow C_6H_6 + 2\ CH_3NHCH_3$	209.0
19	$C_6H_5NHNH_2 + CH_4 + CH_3CH_3 \rightarrow C_6H_5CH_3 + 2\ CH_3NH_2$	206.6
20	$C_6H_5NHNH_2 + 2\ H_2O \rightarrow C_6H_6 + 2\ NH_2OH$	207.6

average of 10 reactions (11-20) with different species 207.6

average of all 20 reactions 208.3

1-methyl-1-phenylhydrazine: $C_6H_5N(CH_3)NH_2$ (12)

atomization reaction 208.9

reactions with $C_6H_5NHNH_2$

1	$C_6H_5N(CH_3)NH_2 + CH_4 \rightarrow C_6H_5NHNH_2 + CH_3CH_3$	203.2
2	$C_6H_5N(CH_3)NH_2 + CH_3CH_3 \rightarrow C_6H_5NHNH_2 + CH_3CH_2CH_3$	203.1
3	$C_6H_5N(CH_3)NH_2 + CH_3CH_2CH_3 \rightarrow C_6H_5NHNH_2 + CH_3CH(CH_3)_2$	202.5
4	$C_6H_5N(CH_3)NH_2 + 2\ H_2C=CH_2 \rightarrow C_6H_5NHNH_2 + CH_3CH=CH_2$	203.1
5	$C_6H_5N(CH_3)NH_2 + CH_3NH_2 \rightarrow C_6H_5NHNH_2 + CH_3NHCH_3$	204.9
6	$C_6H_5N(CH_3)NH_2 + CH_3OH \rightarrow C_6H_5NHNH_2 + CH_3OCH_3$	204.3
7	$C_6H_5N(CH_3)NH_2 + C_6H_6 \rightarrow C_6H_5NHNH_2 + C_6H_5CH3$	204.2
8	$C_6H_5N(CH_3)NH_2 + C_6H_5NH_2 \rightarrow C_6H_5NHNH_2 + C_6H_5NHCH_3$	201.8

average of 8 reactions (1-8) with $C_6H_5NHNH_2$ 203.4

reactions with CH_3NHNH_2

9	$C_6H_5N(CH_3)NH_2 + CH_4 \rightarrow CH_3NHNH_2 + C_6H_5CH_3$	206.7
10	$C_6H_5N(CH_3)NH_2 + CH_3OH \rightarrow CH_3NHNH_2 + C_6H_5CH_2OH$	207.7
11	$C_6H_5N(CH_3)NH_2 + CH_3OH \rightarrow CH_3NHNH_2 + C_6H_5OCH_3$	206.8
12	$C_6H_5N(CH_3)NH_2 + NH_3 \rightarrow CH_3NHNH_2 + C_6H_5NH_2$	209.2
13	$C_6H_5N(CH_3)NH_2 + H_2C=CH_2 \rightarrow CH_3NHNH_2 + C_6H_5CH=CH_2$	206.5

average of 5 reactions (1-5) with CH_3NHNH_2 207.4

reactions with $(CH_3)_2NNH_2$

14	$C_6H_5N(CH_3)NH_2 + CH_3CH_3 \rightarrow (CH_3)_2NNH_2 + C_6H_5CH_3$	208.4
15	$C_6H_5N(CH_3)NH_2 + CH_3CH_2OH \rightarrow (CH_3)_2NNH_2 + C_6H_5CH_2OH$	210.5
16	$C_6H_5N(CH_3)NH_2 + CH_3CH_2OH \rightarrow (CH_3)_2NNH_2 + C_6H_5OCH_3$	209.6
17	$C_6H_5N(CH_3)NH_2 + CH_3NH_2 \rightarrow (CH_3)_2NNH_2 + C_6H_5NH_2$	208.6
18	$C_6H_5N(CH_3)NH_2 + CH_3CH=CH_2 \rightarrow (CH_3)_2NNH_2 + C_6H_5CH=CH_2$	208.2

average of 5 reactions (14-18) with $(CH_3)_2NNH_2$ 209.1

reactions with different species

19	$C_6H_5N(CH_3)NH_2 + CH_4 \rightarrow C_6H_5NH_2 + CH_3NHCH_3$	207.2
20	$C_6H_5N(CH_3)NH_2 + CH_4 \rightarrow C_6H_5NHCH_3 + CH_3NH_2$	204.1
21	$C_6H_5N(CH_3)NH_2 + CH_4 \rightarrow C_6H_5N(CH_3)_2 + NH_3$	205.5
22	$C_6H_5N(CH_3)NH_2 + CH_3CH_3 \rightarrow H_2NCH_2CH_2NH_2 + C_6H_5CH_3$	205.8
23	$C_6H_5N(CH_3)NH_2 + CH_3CH_3 \rightarrow C_6H_5NHCH_2CH_3 + CH_3NH_2$	208.8
24	$C_6H_5N(CH_3)NH_2 \rightarrow NH{=}NH + C_6H_5CH_3$	205.7
25	$C_6H_5N(CH_3)NH_2 + H_2O \rightarrow C_6H_5NHCH_3 + NH_2OH$	205.2
26	$C_6H_5N(CH_3)NH_2 + 2\ CH_3CH_3 \rightarrow C_6H_5CH_3 + 2\ CH_3NHCH_3$	208.7
27	$C_6H_5N(CH_3)NH_2 + 2\ CH_4 \rightarrow C_6H_5CH_3 + 2\ CH_3NH_2$	205.2
28	$C_6H_5N(CH_3)NH_2 + 2\ H_2O \rightarrow C_6H_5CH_3 + 2\ NH_2OH$	207.2
	average of 10 reactions (19-28) with different species	**206.3**
	average of 20 reactions (9-28) without $C_6H_5NHNH_2$	**207.3**

1,2-diphenylhydrazine: $C_6H_5NHNHC_6H_5$ (13)

atomization reaction 319.4

reactions with $C_6H_5N(CH_3)NH_2$

1	$C_6H_5NHNHC_6H_5 + CH_4 \rightarrow C_6H_5N(CH_3)NH_2 + C_6H_6$	319.7
2	$C_6H_5NHNHC_6H_5 + CH_3CH_3 \rightarrow C_6H_5N(CH_3)NH_2 + C_6H_5CH_3$	320.7
3	$C_6H_5NHNHC_6H_5 + CH_3CH_2CH_3 \rightarrow C_6H_5N(CH_3)NH_2 + C_6H_5CH_2CH_3$	322.8
4	$C_6H_5NHNHC_6H_5 + (CH_3)_2CHCH_3 \rightarrow C_6H_5N(CH_3)NH_2 + C_9H_{12}$ (1,3,5trimethylbenzene)	322.6
5	$C_6H_5NHNHC_6H_5 + CH_3CH{=}CH_2 \rightarrow C_6H_5N(CH_3)NH_2 + C_6H_5CH{=}CH_2$	320.6
6	$C_6H_5NHNHC_6H_5 + CH_3OCH_3 \rightarrow C_6H_5N(CH_3)NH_2 + C_6H_5OCH_3$	319.6
7	$C_6H_5NHNHC_6H_5 + CH_3CH_2OH \rightarrow C_6H_5N(CH_3)NH_2 + C_6H_5CH_2OH$	322.9
8	$C_6H_5NHNHC_6H_5 + CH_3NH_2 \rightarrow C_6H_5N(CH_3)NH_2 + C_6H_5NH_2$	321.0
9	$C_6H_5NHNHC_6H_5 + CH_3NHCH_3 \rightarrow C_6H_5N(CH_3)NH_2 + C_6H_5NHCH_3$	317.9
10	$C_6H_5NHNHC_6H_5 + (CH_3)_3N \rightarrow C_6H_5N(CH_3)NH_2 + C_6H_5NHCH_2CH_3$	320.7
	average of 10 reactions (1-10) with $C_6H_5N(CH_3)NH_2$	**320.9**

reactions with CH_3NHNH_2

11	$C_6H_5NHNHC_6H_5 + CH_4 + CH_3CH_3 \rightarrow CH_3NHNH_2 + 2\ C_6H_5CH_3$	316.7
12	$C_6H_5NHNHC_6H_5 + CH_3OH + CH_3OCH_3 \rightarrow CH_3NHNH_2 + 2\ C_6H_5OCH_3$	315.6
13	$C_6H_5NHNHC_6H_5 + CH_3OH + CH_3OCH_3 \rightarrow CH_3NHNH_2 + 2\ C_6H_5CH_2OH$	317.4
14	$C_6H_5NHNHC_6H_5 + CH_3CH_3 + CH_3NH_2 \rightarrow CH_3NHNH_2 + C_6H_5NHCH_3 + C_6H_5CH_3$	315.6
15	$C_6H_5NHNHC_6H_5 + CH_3CH{=}CH_2 + CH_4 \rightarrow CH_3NHNH_2 + C_6H_5CH{=}CH_2 + C_6H_5CH_3$	316.6
	average of 5 reactions (11-15) with CH_3NHNH_2	**316.4**

reactions with $(CH_3)_2NNH_2$

16	$C_6H_5NHNHC_6H_5 + 2\ CH_3CH_3 \rightarrow (CH_3)_2NNH_2 + 2\ C_6H_5CH_3$	318.3
17	$C_6H_5NHNHC_6H_5 + 2\ CH_3OCH_3 \rightarrow (CH_3)_2NNH_2 + 2\ C_6H_5OCH_3$	316.1
18	$C_6H_5NHNHC_6H_5 + 2\ CH_3OCH_3 \rightarrow (CH_3)_2NNH_2 + 2\ C_6H_5CH_2OH$	317.9
19	$C_6H_5NHNHC_6H_5 + CH_3CH_2CH_3 + CH_3NH_2 \rightarrow (CH_3)_2NNH_2 + C_6H_5NHCH_3 + C_6H_5CH_3$	317.3
20	$C_6H_5NHNHC_6H_5 + H_2C{=}CH_2 + CH_3CH_3 \rightarrow (CH_3)_2NNH_2 + C_6H_5CH{=}CH_2 + C_6H_5CH_3$	318.2
	average of 5 reactions (16-20) with $(CH3)_2NNH_2$	**317.5**

reactions with different species

21	$C_6H_5NHNHC_6H_5 + 2\ CH_4 \rightarrow 2\ C_6H_5NH_2 + CH_3CH_3$	315.7
22	$C_6H_5NHNHC_6H_5 + CH_3CH_3 \rightarrow 2\ C_6H_5NHCH_3$	313.0
23	$C_6H_5NHNHC_6H_5 + CH_3CH_2CH_2CH_3 \rightarrow 2\ C_6H_5N(CH_3)_2$	319.9
24	$C_6H_5NHNHC_6H_5 + CH_3CH_2CH_2CH_3 \rightarrow 2\ C_6H_5NHCH_2CH_3$	322.1
25	$C_6H_5NHNHC_6H_5 + CH_4 + CH_3CH_2CH_3 \rightarrow H_2NCH_2CH_2NH_2 + 2\ C_6H_5CH_3$	315.8
26	$C_6H_5NHNHC_6H_5 + CH_3CH_3 \rightarrow NH{=}NH + 2\ C_6H_5CH_3$	315.7

27	$C_6H_5NHNHC_6H_5 + CH_3CH_3 + 2\ H_2O \rightarrow 2\ C_6H_5CH_3 + 2\ NH_2OH$	317.2
28	$C_6H_5NHNHC_6H_5 + 3\ CH_3CH_3 \rightarrow 2\ C_6H_5CH_3 + 2\ CH_3NHCH_3$	318.6
29	$C_6H_5NHNHC_6H_5 + 2\ CH_4 + CH_3CH_3 \rightarrow 2\ C_6H_5CH_3 + 2\ CH_3NH_2$	315.1
30	$C_6H_5NHNHC_6H_5 + 2\ HCN + CH_3CH_3 \rightarrow 2\ C_6H_5CH_3 + 2\ NCNH_2$	314.7
	average of 10 reactions (21-30) with different species	**316.8**
	average of 20 reactions (11-30) without $C_6H_5N(CH_3)NH_2$	**316.9**

1,1-diphenylhydrazine: $(C_6H_5)_2NNH_2$ (14)

atomization reaction		335.8
reactions with CH_3NHNH_2		
1	$(C_6H_5)_2NNH_2 + CH_4 + CH_3CH_3 \rightarrow CH_3NHNH_2 + 2\ C_6H_5CH_3$	333.2
2	$(C_6H_5)_2NNH_2 + CH_3OH + CH_3OCH_3 \rightarrow CH_3NHNH_2 + 2\ C_6H_5OCH_3$	332.1
3	$(C_6H_5)_2NNH_2 + CH_3OH + CH_3OCH_3 \rightarrow CH_3NHNH_2 + 2\ C_6H_5CH_2OH$	333.9
4	$(C_6H_5)_2NNH_2 + CH_3CH_3 + CH_3NH_2 \rightarrow CH_3NHNH_2 + C_6H_5NHCH_3 + C_6H_5CH_3$	332.1
5	$(C_6H_5)_2NNH_2 + CH_3CH{=}CH_2 + CH_4 \rightarrow CH_3NHNH_2 + C_6H_5CH{=}CH_2 + C_6H_5CH_3$	333.0
	average of 5 reactions (1-5) with CH_3NHNH_2	**332.9**
reactions with $(CH_3)_2NNH_2$		
6	$(C_6H_5)_2NNH_2 + 2\ CH_3CH_3 \rightarrow (CH_3)_2NNH_2 + 2\ C_6H_5CH_3$	334.8
7	$(C_6H_5)_2NNH_2 + 2\ CH_3OCH_3 \rightarrow (CH_3)_2NNH_2 + 2\ C_6H_5OCH_3$	332.6
8	$(C_6H_5)_2NNH_2 + 2\ CH_3OCH_3 \rightarrow (CH_3)_2NNH_2 + 2\ C_6H_5CH_2OH$	334.4
9	$(C_6H_5)_2NNH_2 + CH_3CH_2CH_3 + CH_3NH_2 \rightarrow (CH_3)_2NNH_2 + C_6H_5NHCH_3 + C_6H_5CH_3$	333.8
10	$(C_6H_5)_2NNH_2 + H_2C{=}CH_2 + CH_3CH_3 \rightarrow (CH_3)_2NNH_2 + C_6H_5CH{=}CH_2 + C_6H_5CH_3$	334.6
	average of 5 reactions (6-10) with $(CH_3)_2NNH_2$	**334.0**
reactions with different species		
11	$(C_6H_5)_2NNH_2 + 2\ CH_4 \rightarrow 2\ C_6H_5NH_2 + CH_3CH_3$	332.2
12	$(C_6H_5)_2NNH_2 + CH_3CH_3 \rightarrow 2\ C_6H_5NHCH_3$	329.5
13	$(C_6H_5)_2NNH_2 + CH_3CH_2CH_2CH_3 \rightarrow 2\ C_6H_5N(CH_3)_2$	336.4
14	$(C_6H_5)_2NNH_2 + CH_3CH_2CH_2CH_3 \rightarrow 2\ C_6H_5NHCH_2CH_3$	338.5
15	$(C_6H_5)_2NNH_2 + CH_4 + CH_3CH_2CH_3 \rightarrow H_2NCH_2CH_2NH_2 + 2\ C_6H_5CH_3$	332.2
16	$(C_6H_5)_2NNH_2 + CH_3CH_3 \rightarrow NH{=}NH + 2\ C_6H_5CH_3$	332.2
17	$(C_6H_5)_2NNH_2 + CH_3CH_3 + 2\ H_2O \rightarrow 2\ C_6H_5CH_3 + 2\ NH_2OH$	333.7
18	$(C_6H_5)_2NNH_2 + 3\ CH_3CH_3 \rightarrow 2\ C_6H_5CH_3 + 2\ CH_3NHCH_3$	335.1
19	$(C_6H_5)_2NNH_2 + 2\ CH_4 + CH_3CH_3 \rightarrow 2\ C_6H_5CH_3 + 2\ CH_3NH_2$	331.6
20	$(C_6H_5)_2NNH_2 + 2\ HCN + CH_3CH_3 \rightarrow 2\ C_6H_5CH_3 + 2\ NCNH_2$	331.2
	average of 10 reactions (11-20) with different species	**333.3**
	average of all 20 reactions	**333.4**

triphenylhydrazine: $(C_6H_5)_2NNHC_6H_5$ (15)[b]

atomization reaction		429.0
reactions with CH_3NHNH_2 and $(CH_3)_2NNH_2$		
1	$(C_6H_5)_2NNHC_6H_5 + 2\ CH_4 + CH_3CH_3 \rightarrow CH_3NHNH_2 + 3\ C_6H_5CH_3$	440.0
2	$(C_6H_5)_2NNHC_6H_5 + CH_4 + 2\ CH_3CH_3 \rightarrow (CH_3)_2NNH_2 + 3\ C_6H_5CH_3$	440.6
	average of 2 reactions with CH_3NHNH_2 and $(CH_3)_2NNH_2$	**440.3**
reactions with different species from ATcT		
3	$(C_6H_5)_2NNHC_6H_5 + CH_4 + CH_3CH_3 \rightarrow NH{=}NH + 3\ C_6H_5CH_3$	441.0
4	$(C_6H_5)_2NNHC_6H_5 + CH_4 + 3\ CH_3CH_3 \rightarrow 2\ CH_3NHCH_3 + 3\ C_6H_5CH_3$	440.7

5	$(C_6H_5)_2NNHC_6H_5 + 4\ CH_4 \rightarrow 2\ CH_3NHCH_3 + 3\ C_6H_6$	439.4
6	$(C_6H_5)_2NNHC_6H_5 + 3\ CH_4 + CH_3CH_3 \rightarrow 2\ CH_3NH_2 + 3\ C_6H_5CH_3$	439.2
7	$(C_6H_5)_2NNHC_6H_5 + 5\ CH_4 \rightarrow 2\ CH_3NH_2 + 3\ C_6H_6 + CH_3CH_2CH_3$	437.9
8	$(C_6H_5)_2NNHC_6H_5 + 2\ CH_3OH + 3\ CH_4 \rightarrow 3\ C_6H_5CH_3 + 2\ NH_2OH + CH_3CH_3$	436.8
	average of 6 reactions with different species	**439.2**
	average of all 8 reactions	**439.5**

tetraphenylhydrazine: $(C_6H_5)_2NN(C_6H_5)_2$ (16)[b]

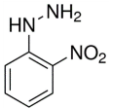
atomization reaction 529.9

reactions with CH_3NHNH_2 and $(CH_3)_2NNH_2$

1	$(C_6H_5)_2NN(C_6H_5)_2 + 3\ CH_4 + CH_3CH_3 \rightarrow CH_3NHNH_2 + 4\ C_6H_5CH_3$	545.2
2	$(C_6H_5)_2NN(C_6H_5)_2 + 2\ CH_4 + 2\ CH_3CH_3 \rightarrow (CH_3)_2NNH_2 + 4\ C_6H_5CH_3$	545.9
	average of 2 reactions with CH_3NHNH_2 and $(CH_3)_2NNH_2$	**545.6**

reactions with different species from ATcT

3	$(C_6H_5)_2NN(C_6H_5)_2 + 2\ CH_4 + CH_3CH_3 \rightarrow NH{=}NH + 4\ C_6H_5CH_3$	546.2
4	$(C_6H_5)_2NN(C_6H_5)_2 + 2\ CH_4 + 3\ CH_3CH_3 \rightarrow 2\ CH_3NHCH_3 + 4\ C_6H_5CH_3$	546.0
5	$(C_6H_5)_2NN(C_6H_5)_2 + 6\ CH_4 \rightarrow 2\ CH3NHCH3 + 4\ C_6H_6 + CH_3CH_3$	544.2
6	$(C_6H_5)_2NN(C_6H_5)_2 + 4\ CH_4 + CH_3CH_3 \rightarrow 2\ CH_3NH_2 + 4\ C_6H_5CH_3$	544.4
7	$(C_6H_5)_2NN(C_6H_5)_2 + 6\ CH_4 \rightarrow 2\ CH_3NH_2 + 4\ C_6H_6 + CH_3CH_2CH_2CH_3$	543.0
8	$(C_6H_5)_2NN(C_6H_5)_2 + 2\ CH_3OH + 4\ CH_4 \rightarrow 4\ C_6H_5CH_3 + 2\ NH_2OH + CH_3CH_3$	542.0
	average of 6 reactions with different species	**544.3**
	average of all 8 reactions	**544.6**

2-nitrophenylhydrazine:  **(17)**

atomization reaction 178.9

reactions with different species

1	$2\text{-}NO_2\text{-}C_6H_4\text{-}NHNH_2 + \bullet H \rightarrow C_6H_5NO_2 + \bullet NHNH_2$	186.1
2	$2\text{-}NO_2\text{-}C_6H_4\text{-}NHNH_2 + 2\ CH_4 \rightarrow CH_3NO_2 + C_6H_6 + CH_3NHNH_2$	182.8
3	$2\text{-}NO_2\text{-}C_6H_4\text{-}NHNH_2 + CH_4 \rightarrow C_6H_5NO_2 + CH_3NHNH_2$	186.0
4	$2\text{-}NO_2\text{-}C_6H_4\text{-}NHNH_2 + CH_4 + CH_3CH_3 \rightarrow CH_3NO_2 + C_6H_6 + (CH_3)_2NHNH_2$	184.5
5	$2\text{-}NO_2\text{-}C_6H_4\text{-}NHNH_2 + CH_3CH_3 \rightarrow C_6H_5NO_2 + (CH_3)_2NHNH_2$	187.6
6	$2\text{-}NO_2\text{-}C_6H_4\text{-}NHNH_2 \rightarrow C_6H_5NO_2 + HN{=}NH$	185.0
7	$2\text{-}NO_2\text{-}C_6H_4\text{-}NHNH_2 + CH_3CH_3 \rightarrow CH_3NO_2 + C_6H_5CH_3 + HN{=}NH$	182.9
8	$2\text{-}NO_2\text{-}C_6H_4\text{-}NHNH_2 + CH_4 \rightarrow C_6H_5NH_2 + CH_3NHNO_2$	182.7
	average of 8 reactions	**184.7**

4,4'-dinitrohydrazobenzene: $O_2NC_6H_4NHNHC_6H_4NO_2$ (18)[b]

atomization reaction 267.4

reactions with CH_3NHNH_2 and $(CH_3)_2NNH_2$

1	$O_2NC_6H_4NHNHC_6H_4NO_2 + 3\ CH_4 \rightarrow 2\ C_6H_5NO_2 + CH_3NHNH_2 + CH_3CH_3$	279.3
2	$O_2NC_6H_4NHNHC_6H_4NO_2 + 5\ CH_4 \rightarrow 2\ CH_3NO_2 + CH_3NHNH_2 + 2\ C_6H_6 + CH_3CH_3$	276.1
3	$O_2NC_6H_4NHNHC_6H_4NO_2 + 2\ CH_4 \rightarrow 2\ C_6H_5NO_2 + (CH_3)_2NNH_2$	279.9
4	$O_2NC_6H_4NHNHC_6H_4NO_2 + 4\ CH_4 \rightarrow 2\ CH_3NO_2 + (CH_3)_2NNH_2 + 2\ C_6H_6$	276.8
	average of 4 reactions with CH_3NHNH_2 and $(CH_3)_2NNH_2$	**278.0**

reactions with different species

5	$O_2NC_6H_4NHNHC_6H_4NO_2 + 2\ CH_4 \rightarrow 2\ C_6H_5NO_2 + HN{=}NH + CH_3CH_3$	280.3
6	$O_2NC_6H_4NHNHC_6H_4NO_2 + 2\ CH_4 + CH_3CH_3 \rightarrow 2\ C_6H_5NO_2 + 2\ CH_3NHCH_3$	280.1
7	$O_2NC_6H_4NHNHC_6H_4NO_2 + 4\ CH_4 \rightarrow 2\ CH_3NO_2 + HN{=}NH + 2\ C_6H_6 + CH_3CH_3$	277.1
8	$O_2NC_6H_4NHNHC_6H_4NO_2 + 4\ CH_4 + CH_3CH_3 \rightarrow 2\ CH_3NO_2 + 2\ CH_3NHCH_3 + 2\ C_6H_6$	276.9

average of 4 reactions with different species **278.6**

average of all 8 reactions **278.3**

hydrazinecarboxamide: $H_2NC(O)NHNH_2$ (19)

atomization reaction -115.5

reactions with different species

1	$H_2NC(O)NHNH_2 + CH_3CH_3 \rightarrow H_2NC(O)NH_2 + CH_3NHCH_3$	-118.3
2	$H_2NC(O)NHNH_2 + CH_3SH \rightarrow H_2NC(S)NHNH_2 + CH_3OH$	-112.4
3	$H_2NC(O)NHNH_2 + H_2S \rightarrow H_2NC(S)NHNH_2 + H_2O$	-113.7
4	$H_2NC(O)NHNH_2 + CH_3CH_2SH \rightarrow H_2NC(S)NHNH_2 + CH_3CH_2OH$	-115.3
5	$H_2NC(O)NHNH_2 + CH_3SH + CH_4 \rightarrow H_2NC(S)NH_2 + CH_3OH + CH_3NH_2$	-111.6
6	$H_2NC(O)NHNH_2 + H_2S + CH_3CH_3 \rightarrow H_2NC(S)NH_2 + H_2O + CH_3NHCH_3$	-111.1
7	$H_2NC(O)NHNH_2 + CH_3CH_2SH + CH_4 \rightarrow H_2NC(S)NH_2 + CH_3CH_2OH + CH_3NH_2$	-114.5
8	$H_2NC(O)NHNH_2 + 2\ CH_3CH_3 \rightarrow CH_3NHNH_2 + CH_3NH_2 + CH_3C(O)CH_3$	-116.8
9	$H_2NC(O)NHNH_2 + 2\ CH_4 \rightarrow CH_3NHNH_2 + CH_3NH_2 + HC(O)H$	-115.0
10	$H_2NC(O)NHNH_2 + 2\ CH_3CH_3 \rightarrow CH_3NHNH_2 + CH_3NHCH_3 + CH_3C(O)H$	-114.7
11	$H_2NC(O)NHNH_2 + 2\ CH_3CH_3 \rightarrow (CH_3)_2NNH_2 + CH_3NH_2 + CH_3C(O)H$	-114.9
12	$H_2NC(O)NHNH_2 + 2\ CH_4 \rightarrow (CH_3)_2NNH_2 + NH_3 + HC(O)H$	-115.5
13	$H_2NC(O)NHNH_2 + 2\ CH_3CH_3 \rightarrow (CH_3)_2NNH_2 + CH_3NHCH_3 + HC(O)H$	-111.6
14	$H_2NC(O)NHNH_2 + CH_4 + CH_3CH_3 \rightarrow CH_3C(O)NH_2 + 2\ CH_3NH_2$	-120.7
15	$H_2NC(O)NHNH_2 + CH_3CH_3 \rightarrow HC(O)NH_2 + H_2NCH_2CH_2NH_2$	-117.4
16	$H_2NC(O)NHNH_2 + C_4H_4O$ [furan] $\rightarrow C_5H_6N_2O_2$ [fur-C(O)NHNH$_2$] $+ NH_3$	-115.0
17	$H_2NC(O)NHNH_2 + C_5H_4O_2$ [3-fur-C(O)H] $\rightarrow C_5H_6N_2O_2$ [fur-C(O)NHNH$_2$] $+ HC(O)NH_2$	-115.3
18	$H_2NC(O)NHNH_2 + C_6H_6O_2$ [fur-C(O)CH$_3$] $\rightarrow C_5H_6N_2O_2$ [fur-C(O)NHNH$_2$] $+ CH_3C(O)NH_2$	-117.5

average of 18 reactions **-115.1**

carbohydrazide: $H_2NNHC(O)NHNH_2$ (20)

atomization reaction 4.6

reactions with different species

1	$H2NNHC(O)NHNH2 + H_2S \rightarrow H_2NC(S)NH_2 + NH{=}NH + H_2O$	6.5
2	$H_2NNHC(O)NHNH_2 + H_2 + CH_3SH \rightarrow H_2NC(S)NH_2 + H_2NNH_2 + CH_3OH$	3.7
3	$H_2NNHC(O)NHNH_2 + CH_3CH_3 + CH_3SCH_3 \rightarrow H_2NC(S)NH_2 + H_2NCH_2CH_2NH_2 + CH_3OCH_3$	6.5
4	$H_2NNHC(O)NHNH_2 + H_2S + CH_3CH_3 \rightarrow H_2NC(S)NHNH_2 + CH_3NHCH_3 + H_2O$	6.9
5	$H_2NNHC(O)NHNH_2 + CH_3SH + CH_4 \rightarrow H_2NC(S)NHNH_2 + CH_3NH_2 + CH_3OH$	6.5
6	$H_2NNHC(O)NHNH_2 + CH_3SCH_3 + CH_4 \rightarrow H_2NC(S)NHNH_2 + CH_3NH_2 + CH_3OCH_3$	5.1
7	$H_2NNHC(O)NHNH_2 + 2\ CH_3CH_3 \rightarrow 2\ CH_3NHNH_2 + CH_3C(O)CH_3$	3.6
8	$H_2NNHC(O)NHNH_2 + 2\ CH_4 \rightarrow 2\ CH_3NHNH_2 + HC(O)H$	5.4
9	$H_2NNHC(O)NHNH_2 + CH_4 + CH_3CH_3 \rightarrow 2\ CH_3NHNH_2 + CH_3C(O)H$	3.9
10	$H_2NNHC(O)NHNH_2 + 2\ CH_3CH_3 \rightarrow 2\ (CH_3)_2NNH_2 + HC(O)H$	8.6
11	$H_2NNHC(O)NHNH_2 + 2\ CH_3CH_2CH_3 \rightarrow 2\ (CH_3)_2NNH_2 + CH_3C(O)CH_3$	7.0
12	$H_2NNHC(O)NHNH_2 + CH_3CH_3 + CH_3CH_2CH_3 \rightarrow 2\ (CH_3)_2NNH_2 + CH_3C(O)H$	7.2
13	$H_2NNHC(O)NHNH_2 + 4\ CH_3CH_3 \rightarrow CH_3C(O)CH_3 + 2\ CH_3NH_2 + 2\ CH_3NHCH_3$	4.0
14	$H_2NNHC(O)NHNH_2 + 4\ CH_3CH_3 \rightarrow HC(O)H + 4\ CH_3NHCH_3$	9.3
15	$H_2NNHC(O)NHNH_2 + 4\ CH_3CH_3 \rightarrow CH_3C(O)H + CH_3NH_2 + 3\ CH_3NHCH_3$	6.1
16	$H_2NNHC(O)NHNH_2 + 3\ CH_3CH_3 \rightarrow CH_3C(O)NH_2 + CH_3NH_2 + 2\ CH_3NHCH_3$	1.6
17	$H_2NNHC(O)NHNH_2 + 3\ CH_3CH_3 \rightarrow HC(O)NH_2 + 3\ CH_3NHCH_3$	6.1

	average of 17 reactions	**5.8**

1,2-hydrazinedicarboxaldehyde: HC(O)NHNHC(O)H (21)

atomization reaction		-217.1
reactions with different species		
1	$HC(O)NHNHC(O)H + 2\ CH_4 \rightarrow 2\ HC(O)NH_2 + CH_3CH_3$	-217.8
2	$HC(O)NHNHC(O)H + 2\ C_6H_5CH_3 \rightarrow 2\ C_6H_5C(O)NH_2 + CH_3CH_3$	-218.1
3	$HC(O)NHNHC(O)H \rightarrow 2\ HC(O)H + N_2$	-216.0
4	$HC(O)NHNHC(O)H + H_2 \rightarrow 2\ HC(O)H + NH{=}NH$	-215.1
5	$HC(O)NHNHC(O)H + 2\ CH_4 + CH_3CH_3 \rightarrow 2\ HC(O)H + 2\ CH_3NHCH_3$	-211.3
6	$HC(O)NHNHC(O)H + 3\ CH_4 \rightarrow 2\ HC(O)H + CH_3NHNH_2 + CH_3CH_3$	-213.3
7	$HC(O)NHNHC(O)H + 2\ CH_4 \rightarrow 2\ HC(O)H + (CH_3)_2NNH_2$	-211.7
8	$HC(O)NHNHC(O)H \rightarrow HC(O)C(O)H + NH{=}NH$	-215.4
9	$HC(O)NHNHC(O)H + 2\ CH_3CH_3 \rightarrow HC(O)C(O)H + 2\ CH_3NHCH_3$	-212.4
10	$HC(O)NHNHC(O)H + CH_4 \rightarrow HC(O)C(O)H + CH_3NHNH_2$	-214.3
11	$HC(O)NHNHC(O)H + CH_3CH_3 \rightarrow HC(O)C(O)H + (CH_3)_2NNH_2$	-212.7
12	$HC(O)NHNHC(O)H + CH_3CH_3 \rightarrow 2\ CH_3C(O)H + NH{=}NH$	-217.3
13	$HC(O)NHNHC(O)H + 3\ CH_3CH_3 \rightarrow 2\ CH_3C(O)H + 2\ CH_3NHCH_3$	-214.3
14	$HC(O)NHNHC(O)H + CH_3CH_3 + CH_4 \rightarrow 2\ CH_3C(O)H + CH_3NHNH_2$	-216.3
15	$HC(O)NHNHC(O)H + 2\ CH_3CH_3 \rightarrow 2\ CH_3C(O)H + (CH_3)_2NNH_2$	-214.7
16	$HC(O)NHNHC(O)H \rightarrow H_2NC(O)C(O)NH_2$	-216.2
	average of 16 reactions	**-214.8**

1,2-diacetylhydrazine: $CH_3C(O)NHNHC(O)CH_3$ (22)

atomization reaction		-318.5
reactions with different species		
1	$CH_3C(O)NHNHC(O)CH_3 + 2\ CH_4 \rightarrow 2\ HC(O)NH_2 + CH_3CH_2CH_2CH_3$	-320.2
2	$CH_3C(O)NHNHC(O)CH_3 + 2\ C_6H_6 \rightarrow 2\ C_6H_5C(O)NH_2 + CH_3CH_3$	-318.6
3	$CH_3C(O)NHNHC(O)CH_3 \rightarrow 2\ CH_3C(O)H + N_2$	-321.7
4	$CH_3C(O)NHNHC(O)CH_3 + CH_3CH_3 \rightarrow 2\ CH_3C(O)CH_3 + NH{=}NH$	-320.6
5	$CH_3C(O)NHNHC(O)CH_3 + 3\ CH_3CH_3 \rightarrow 2\ CH_3C(O)CH_3 + 2\ CH_3NHCH_3$	-317.6
6	$CH_3C(O)NHNHC(O)CH_3 + CH_4 + CH_3CH_3 \rightarrow 2\ CH_3C(O)CH_3 + CH_3NHNH_2$	-319.5
7	$CH_3C(O)NHNHC(O)CH_3 + 2\ CH_3CH_3 \rightarrow 2\ CH_3C(O)CH_3 + (CH_3)_2NNH_2$	-317.9
8	$CH_3C(O)NHNHC(O)CH_3 \rightarrow CH_3C(O)C(O)CH_3 + NH{=}NH$	-318.8
9	$CH_3C(O)NHNHC(O)CH_3 + 2\ CH_3CH_3 \rightarrow CH_3C(O)C(O)CH_3 + 2\ CH_3NHCH_3$	-315.9
10	$CH_3C(O)NHNHC(O)CH_3 + CH_4 \rightarrow CH_3C(O)C(O)CH_3 + CH_3NHNH_2$	-317.8
11	$CH_3C(O)NHNHC(O)CH_3 + CH_3CH_3 \rightarrow CH_3C(O)C(O)CH_3 + (CH_3)_2NNH_2$	-316.2
12	$CH_3C(O)NHNHC(O)CH_3 + 2\ CH_4 \rightarrow 2\ CH_3C(O)H + NH{=}NH + CH_3CH_3$	-320.0
13	$CH_3C(O)NHNHC(O)CH_3 + 2\ CH_4 + CH_3CH_3 \rightarrow 2\ CH_3C(O)H + 2\ CH_3NHCH_3$	-317.0
14	$CH_3C(O)NHNHC(O)CH_3 + 3\ CH_4 \rightarrow 2\ CH_3C(O)H + CH_3NHNH_2 + CH_3CH_3$	-318.9
15	$CH_3C(O)NHNHC(O)CH_3 + 2\ CH_4 \rightarrow 2\ CH_3C(O)H + (CH_3)_2NNH_2$	-317.3
	average of 15 reactions	**-318.5**

1,2-dibenzoylhydrazine: $C_6H_5C(O)NHNHC(O)C_6H_5$ (23)[b]

atomization reaction		-50.3
reactions with different species		
1	$C_6H_5C(O)NHNHC(O)C_6H_5 + 2\ CH_4 \rightarrow 2\ C_6H_5C(O)NH_2 + CH_3CH_3$	-49.7
2	$C_6H_5C(O)NHNHC(O)C_6H_5 + 4\ CH_4 \rightarrow 2\ HC(O)NH_2 + 2\ C_6H_5CH_3 + CH_3CH_3$	-46.4
3	$C_6H_5C(O)NHNHC(O)C_6H_5 + 4\ CH_4 \rightarrow 2\ HC(O)NH_2 + 2\ C_6H_6 + CH_3CH_2CH_2CH_3$	-47.0

4	$C_6H_5C(O)NHNHC(O)C_6H_5 \rightarrow 2\ C_6H_5C(O)H + N_2$	-45.2
5	$C_6H_5C(O)NHNHC(O)C_6H_5 + H_2 \rightarrow 2\ C_6H_5C(O)H + NH{=}NH$	-46.6
6	$C_6H_5C(O)NHNHC(O)C_6H_5 + CH_4 + CH_3CH_3 \rightarrow CH_3NHNH_2 + 2\ C_6H_5C(O)CH_3$	-51.2
7	$C_6H_5C(O)NHNHC(O)C_6H_5 + 2\ CH_3CH_3 \rightarrow (CH_3)_2NNH_2 + 2\ C_6H_5C(O)CH_3$	-50.8
8	$C_6H_5C(O)NHNHC(O)C_6H_5 + CH_4 + CH_3CH_3 \rightarrow CH_3NHNH_2 + C_6H_5C(O)C_6H_5 + CH_3C(O)CH_3$	-46.8
9	$C_6H_5C(O)NHNHC(O)C_6H_5 + 2\ CH_3CH_3 \rightarrow (CH_3)_2NNH_2 + C_6H_5C(O)C_6H_5 + CH_3C(O)CH_3$	-46.3
10	$C_6H_5C(O)NHNHC(O)C_6H_5 + 4\ CH_4 \rightarrow HC(O)C(O)H + 2\ C_6H_5NH_2 + 2\ CH_3CH_3$	-43.1
11	$C_6H_5C(O)NHNHC(O)C_6H_5 + 4\ CH_4 \rightarrow H_2NC(O)C(O)NH_2 + 2\ C_6H_6 + 2\ CH_3CH_3$	-48.2
	average of 11 reactions	**-47.4**

1,2-hydrazinedicarboxamide: $H_2NC(O)NHNHC(O)NH_2$ (24)

atomization reaction -320.1

reactions with different species

1	$H_2NC(O)NHNHC(O)NH_2 + 2\ CH_4 \rightarrow 2\ H_2NC(O)H + HN{=}NH + CH_3CH_3$	-322.7
2	$H_2NC(O)NHNHC(O)NH_2 + 2\ CH_4 + CH_3CH_3 \rightarrow 2\ H_2NC(O)H + 2\ CH_3NHCH_3$	-319.8
3	$H_2NC(O)NHNHC(O)NH_2 + 3\ CH_4 \rightarrow 2\ H_2NC(O)H + CH_3NHNH_2 + CH_3CH_3$	-321.7
4	$H_2NC(O)NHNHC(O)NH_2 + 2\ CH_4 \rightarrow 2\ H_2NC(O)H + (CH_3)_2NNH_2$	-320.1
5	$H_2NC(O)NHNHC(O)NH_2 + 2\ C_6H_5CH_3 \rightarrow 2\ H_2NC(O)C_6H_5 + HN{=}NH + CH_3CH_3$	-323.1
6	$H_2NC(O)NHNHC(O)NH_2 + 2\ C_6H_5CH_3 + CH_3CH_3 \rightarrow 2\ H_2NC(O)C_6H_5 + 2\ CH_3NHCH_3$	-320.1
7	$H_2NC(O)NHNHC(O)NH_2 + 2\ C_6H_6 + CH_3CH_3 \rightarrow 2\ H_2NC(O)C_6H_5 + CH_3NHNH_2 + CH_4$	-319.9
8	$H_2NC(O)NHNHC(O)NH_2 + 2\ C_6H_6 + CH_3CH_2CH_3 \rightarrow 2\ H_2NC(O)C_6H_5 + (CH_3)_2NNH_2 + CH_4$	-318.2
9	$H_2NC(O)NHNHC(O)NH_2 \rightarrow H_2NC(O)C(O)NH_2 + NH{=}NH$	-321.1
10	$H_2NC(O)NHNHC(O)NH_2 + 2\ CH_4 \rightarrow H_2NC(O)C(O)NH_2 + 2\ CH_3NH_2$	-321.7
11	$H_2NC(O)NHNHC(O)NH_2 + CH_4 \rightarrow H_2NC(O)C(O)NH_2 + CH_3NHNH_2$	-320.1
12	$H_2NC(O)NHNHC(O)NH_2 + CH_3CH_3 \rightarrow H_2NC(O)C(O)NH_2 + (CH_3)_2NNH_2$	-318.5
13	$H_2NC(O)NHNHC(O)NH_2 + 2\ CH_4 \rightarrow 2\ HC(O)H + 2\ HN{=}NH + CH_3CH_3$	-319.3
	average of 13 reactions	**-320.5**

oxalyldihydrazide: $H_2NNHC(O)C(O)NHNH_2$ (25)

atomization reaction -152.0

reactions with different species

1	$H_2NNHC(O)C(O)NHNH_2 \rightarrow HC(O)C(O)H + 2\ NH{=}NH$	-150.2
2	$H_2NNHC(O)C(O)NHNH_2 + 2\ CH_4 \rightarrow HC(O)C(O)H + 2\ CH_3NHNH_2$	-147.0
3	$H_2NNHC(O)C(O)NHNH_2 + 2\ CH_3CH_3 \rightarrow HC(O)C(O)H + 2\ (CH_3)_2NNH_2$	-150.1
4	$H_2NNHC(O)C(O)NHNH_2 + 2\ CH_3CH_3 \rightarrow H_2NC(O)C(O)NH_2 + 2\ CH_3NHCH_3$	-153.6
5	$H_2NNHC(O)C(O)NHNH_2 + 2\ CH_4 \rightarrow H_2NC(O)C(O)NH_2 + 2\ CH_3NH_2$	-152.3
6	$H_2NNHC(O)C(O)NHNH_2 \rightarrow H_2NC(O)C(O)NH_2 + NH{=}NH$	-153.1
7	$H_2NNHC(O)C(O)NHNH_2 + CH_3CH_3 + HOCH_2CH_2OH \rightarrow HOC(O)CH_2CH_2C(O)OH + 2\ HN{=}NH + 2\ CH_4$	-151.2
8	$H_2NNHC(O)C(O)NHNH_2 + 2\ CH4 \rightarrow 2\ HC(O)H + 2\ HN{=}NH + CH3CH3$	-151.2
9	$H_2NNHC(O)C(O)NHNH_2 + 4\ CH4 \rightarrow 2\ HC(O)NH2 + 2\ CH3NH2 + CH3CH3$	-155.3
10	$H_2NNHC(O)C(O)NHNH_2 + 2\ CH4 + CH3CH3 \rightarrow 2\ HC(O)NH2 + 2\ CH3NHCH3$	-151.7
	average of 10 reactions	**-151.6**

hydrazinecarbothioamide: $H_2NC(S)NHNH_2$ (26)

atomization reaction 126.6

reactions with different species

1	$H_2NC(S)NHNH_2 + CH_3CH_3 \rightarrow H_2NC(S)NH_2 + CH_3NHCH_3$	130.8
2	$H_2NC(S)NHNH_2 + H_2O \rightarrow H_2NC(S)NH_2 + NH_2OH$	130.1

3	$H_2NC(S)NHNH_2 + CH_4 \rightarrow H_2NC(S)NH_2 + CH_3NH_2$	129.0
4	$H_2NC(S)NHNH_2 + 3\ CH_4 \rightarrow CH_3NHNH_2 + CH_3SCH_3 + CH_3NH_2$	127.4
5	$H_2NC(S)NHNH_2 + 3\ CH_4 \rightarrow CH_3NHNH_2 + CH_3CH_2SH + CH_3NH_2$	126.7
6	$H_2NC(S)NHNH_2 + 3\ CH_4 \rightarrow (CH_3)_2NNH_2 + CH_3SH + CH_3NH_2$	126.6
7	$H_2NC(S)NHNH_2 + CH_4 + 2\ CH_3CH_3 \rightarrow (CH_3)_2NNH_2 + CH_3SCH_3 + CH_3NHCH_3$	130.8
	average of 7 reactions	**128.8**

thiocarbohydrazide: $H_2NNHC(S)NHNH_2$ (27)

atomization reaction 242.0

reactions with different species

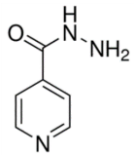
1	$H_2NHNC(S)NHNH_2 + CH_3CH_3 \rightarrow H_2NC(S)NHNH_2 + CH_3NHCH_3$	243.8
2	$H_2NHNC(S)NHNH_2 + H_2O \rightarrow H_2NC(S)NHNH_2 + NH_2OH$	243.0
3	$H_2NHNC(S)NHNH_2 + CH_4 \rightarrow H_2NC(S)NHNH_2 + CH_3NH_2$	242.0
4	$H_2NHNC(S)NHNH_2 + 2\ CH_3CH_3 \rightarrow H_2NC(S)NH_2 + 2\ CH_3NHCH_3$	246.3
5	$H_2NHNC(S)NHNH_2 \rightarrow H_2NC(S)NH_2 + NH{=}NH$	243.4
7	$H_2NHNC(S)NHNH_2 + 2\ CH_4 \rightarrow H_2NC(S)NH_2 + 2\ CH_3NH_2$	242.8
8	$H_2NHNC(S)NHNH_2 + 3\ CH_4 \rightarrow 2\ CH_3NHNH_2 + CH_3SCH_3$	242.8
9	$H_2NHNC(S)NHNH_2 + 3\ CH_4 \rightarrow 2\ CH_3NHNH_2 + CH_3CH_2SH$	242.1
10	$H_2NHNC(S)NHNH_2 + CH_4 + 2\ CH_3CH_3 \rightarrow 2\ (CH_3)_2NNH_2 + CH_3SCH_3$	246.0
11	$H_2NHNC(S)NHNH_2 + 2\ CH_4 + CH_3CH_3 \rightarrow 2\ (CH_3)_2NNH_2 + CH_3SH$	243.6
	average of 11 reactions	**243.6**

2-furancarboxylic acid hydrazide: $C_5H_6N_2O_2$ (28)

atomization reaction -108.6

reactions with different species

1	$C_5H_6N_2O_2$ [fur-C(O)NHNH$_2$] + $CH_3CH_3 \rightarrow C_6H_6O_2$ [fur-C(O)CH$_3$] + HN=NH + CH_4	-109.2
2	$C_5H_6N_2O_2$ [fur-C(O)NHNH$_2$] + $CH_3CH_3 \rightarrow C_6H_6O_2$ [fur-C(O)CH$_3$] + CH_3NHNH_2	-108.1
3	$C_5H_6N_2O_2$ [fur-C(O)NHNH$_2$] + $CH_3CH_2CH_3 \rightarrow C_6H_6O_2$ [fur-C(O)CH$_3$] + $(CH_3)_2NNH_2$	-106.5
4	$C_5H_6N_2O_2$ [fur-C(O)NHNH$_2$] $\rightarrow C_5H_4O_2$ [3-fur-C(O)H] + HN=NH	-108.7
5	$C_5H_6N_2O_2$ [fur-C(O)NHNH$_2$] + $CH_4 \rightarrow C_5H_4O_2$ [3-fur-C(O)H] + CH_3NHNH_2	-107.7
6	$C_5H_6N_2O_2$ [fur-C(O)NHNH$_2$] + $CH_3CH_3 \rightarrow$ C5H4O2 [3-fur-C(O)H] + $(CH_3)_2NNH_2$	-106.1
7	$C_5H_6N_2O_2$ [fur-C(O)NHNH$_2$] + 2 $CH_4 \rightarrow C_4H_4O$ [furan] + HN=NH + HC(O)H + CH_3CH_3	-109.7
8	$C_5H_6N_2O_2$ [fur-C(O)NHNH$_2$] + 3 $CH_4 \rightarrow C_4H_4O$ [furan] + CH_3NHNH_2 + HC(O)H + CH_3CH_3	-108.7
9	$C_5H_6N_2O_2$ [fur-C(O)NHNH$_2$] + 2 $CH_4 \rightarrow C_4H_4O$ [furan] + $(CH_3)_2NNH_2$ + HC(O)H	-107.1
	average of 9 reactions	**-108.0**

4-pyridinecarbonylhydrazine:  **(29)**

atomization reaction 76.0

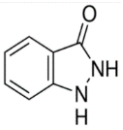
reactions with different species

1	$C_6H_7N_3O$ [pyr-C(O)NHNH$_2$] + $CH_3OH \rightarrow C_6H_5NO_2$ [4-pyr-C(O)OH] + CH_3NHNH_2	73.2
2	$C_6H_7N_3O$ [pyr-C(O)NHNH$_2$] + $CH_3CH_2OH \rightarrow C_6H_5NO_2$ [4-pyr-C(O)OH] + $(CH_3)_2NNH_2$	76.0
3	$C_6H_7N_3O$ [pyr-C(O)NHNH$_2$] + $CH_3OH \rightarrow C_6H_5NO_2$ [4-pyr-C(O)OH] + HN=NH + CH_4	72.2
4	$C_6H_7N_3O$ [pyr-C(O)NHNH$_2$] + $CH_3CH_3 \rightarrow C_6H_6N_2O$ [2-pyr-C(O)NH$_2$] + CH_3NHCH_3	75.6
5	$C_6H_7N_3O$ [pyr-C(O)NHNH$_2$] + $CH_4 \rightarrow C_6H_6N_2O$ [2-pyr-C(O)NH$_2$] + CH_3NH_2	73.8
6	$C_6H_7N_3O$ [pyr-C(O)NHNH$_2$] + 2 $CH_4 \rightarrow C_5H_6N_2$ [pyr-NH$_2$] + $HC(O)NH_2$ + CH_3CH_3	72.1
7	$C_6H_7N_3O$ [pyr-C(O)NHNH$_2$] + 2 $CH_4 \rightarrow C_5H_6N_2$ [pyr-NH$_2$] + HC(O)H + CH_3NHCH_3	75.3
8	$C_6H_7N_3O$ [pyr-C(O)NHNH$_2$] + C_4H_4O [furan] $\rightarrow C_5H_6N_2O_2$ [fur-C(O)NHNH$_2$] + C_5H_5N (pyridine)	79.8

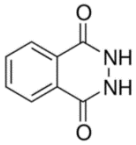
9	$C_6H_7N_3O$ [pyr-C(O)NHNH$_2$] + $C_5H_4O_2$ [3-fur-C(O)H] → $C_5H_6N_2O_2$ [fur-C(O)NHNH$_2$] + $C_6H_5NO_2$ [4-pyr-C(O)OH]	79.1
10	$C_6H_7N_3O$ [pyr-C(O)NHNH$_2$] + 3 CH_4 → C_5H_5N [pyridine] + HC(O)H + CH_3NHNH_2 + CH_3CH_3	77.7
11	$C_6H_7N_3O$ [pyr-C(O)NHNH$_2$] + 2 CH_4 → C_5H_5N [pyridine] + HC(O)H + $(CH_3)_2NHNH_2$	79.3
	average of 11 reactions	**75.8**

benzoic acid hydrazide: $C_6H_5C(O)NHNH_2$ (30)

atomization reaction		16.1
reactions with different species		
1	$C_6H_5C(O)NHNH_2$ + CH_3OH → $C_6H_5C(O)OH$ + CH_3NHNH_2	16.3
2	$C_6H_5C(O)NHNH_2$ + CH_3CH_2OH → $C_6H_5C(O)OH$ + $(CH_3)_2NNH_2$	19.1
3	$C_6H_5C(O)NHNH_2$ + CH_3OH → $C_6H_5C(O)OH$ + HN=NH + CH_4	15.3
4	$C_6H_5C(O)NHNH_2$ + CH_4 → $C_6H_5C(O)H$ + CH_3NHNH_2	15.7
5	$C_6H_5C(O)NHNH_2$ + CH_3CH_3 → $C_6H_5C(O)H$ + $(CH_3)_2NNH_2$	17.4
6	$C_6H_5C(O)NHNH_2$ → $C_6H_5C(O)H$ + HN=NH	14.7
7	$C_6H_5C(O)NHNH_2$ + CH_3CH_3 → $C_6H_5C(O)NH_2$ + CH_3NHCH_3	15.3
8	$C_6H_5C(O)NHNH_2$ + CH_4 → $C_6H_5C(O)NH_2$ + CH_3NH_2	13.5
9	$C_6H_5C(O)NHNH_2$ + 2 CH_4 → $C_6H_5NH_2$ + $HC(O)NH_2$ + CH_3CH_3	14.0
10	$C_6H_5C(O)NHNH_2$ + 2 CH_4 → $C_6H_5NH_2$ + HC(O)H + CH_3NHCH_3	17.2
11	$C_6H_5C(O)NHNH_2$ + 2 CH_4 → $C_6H_5CH_3$ + HC(O)H + CH_3NHNH_2	16.7
12	$C_6H_5C(O)NHNH_2$ + CH_4 + CH_3CH_3 → $C_6H_5CH_3$ + HC(O)H + $(CH_3)_2NNH_2$	18.3
13	$C_6H_5C(O)NHNH_2$ + CH_4 → $C_6H_5CH_3$ + HC(O)H + HN=NH	15.7
14	$C_6H_5C(O)NHNH_2$ + C_4H_4O [furan] → $C_5H_6N_2O_2$ [fur-C(O)NHNH$_2$] + C_6H_6	17.8
	average of 14 reactions	**16.2**

3-indazolinone:  **(31)**

atomization reaction		71.4
reactions with different species		
1	$C_7H_6N_2O$ (3-indazolinone) → $C_7H_6N_2O$ (2-benzimidazolinone)	73.9
2	$C_7H_6N_2O$ (3-indazolinone) + CH_3CH_3 → $C_3H_6N_2O$ (imidazolidin-2-one) + C_6H_6	68.3
3	$C_7H_6N_2O$ (3-indazolinone) + H_2C=$CHCH_3$ → $C_3H_4N_2$ (1*H*-pyrazole) + C_6H_6 + HC(O)H	73.5
4	$C_7H_6N_2O$ (3-indazolinone) + CH_4 → $C_6H_4N_2O$ (benzofurazan) + CH_3CH_3	71.2
5	$C_7H_6N_2O$ (3-indazolinone) + CH_3CH_3 → $C_7H_6N_2$ (1*H*-indazole) + HC(O)H + CH_4	70.7
6	$C_7H_6N_2O$ (3-indazolinone) + CH_3CH_3 → $C_7H_6N_2$ (1*H*-benzimidazole) + HC(O)H + CH_4	72.2
7	$C_7H_6N_2O$ (3-indazolinone) + 2 $CH_3CH_2CH_3$ → C_9H_{10} (indane) + $CH_3C(O)CH_3$ + CH_3NHNH_2	73.5
8	$C_7H_6N_2O$ (3-indazolinone) + CH_3CH_3 + 2 H_2C=CH_2 → C_9H_8 (indene) + $CH_3C(O)CH_3$ + CH_3NHNH_2	73.7
9	$C_7H_6N_2O$ (3-indazolinone) + $CH_3CH_2CH_2CH_2CH_3$ → C_9H_{10} (indane) + $CH_3C(O)CH_3$ + NH=NH	71.7
10	$C_7H_6N_2O$ (3-indazolinone) + CH_3CH=CH_2 + H_2C=CH_2 → C_9H_8 (indene) + $CH_3C(O)CH_3$ + NH=NH	72.7
11	$C_7H_6N_2O$ (3-indazolinone) + $CH_3CH_2CH_3$ → C_9H_{10} (indane) + $H_2NC(O)NH_2$	70.1
12	$C_7H_6N_2O$ (3-indazolinone) + CH_3CH=CH_2 → C_9H_8 (indene) + $H_2NC(O)NH_2$	69.4
	average of 12 reactions	**71.7**

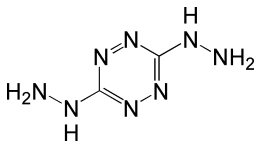
phthalhydrazide:  **(32)**

atomization reaction		-99.8
reactions with different species		
1	$C_8H_6N_2O_2$ (phthalhydrazide) + 4 CH_4 → HC(O)NHNHC(O)H + C_6H_6 + 2 CH_3CH_3	-98.2
2	$C_8H_6N_2O_2$ (phthalhydrazide) + 2 CH_4 + CH_3CH_3 → C_6H_6 + HN=NH + 2 $CH_3C(O)CH_3$	-99.8

3	$C_8H_6N_2O_2$ (phthalhydrazide) + 3 CH_4 + CH_3CH_3 → C_6H_6 + CH_3NHNH_2 + 2 $CH_3C(O)CH_3$	-98.7
4	$C_8H_6N_2O_2$ (phthalhydrazide) + 2 CH_4 + 2 CH_3CH_3 → C_6H_6 + $(CH_3)_2NNH_2$ + 2 $CH_3C(O)CH_3$	-97.1
5	$C_8H_6N_2O_2$ (phthalhydrazide) + 2 $H_2C{=}CH_2$ → $C_4H_4N_2$ (pyrazine) + C_6H_6 + 2 HC(O)H	-96.1
6	$C_8H_6N_2O_2$ (phthalhydrazide) + $H_2C{=}CH_2$ → $C_4H_4N_2O_2$ (uracil) + C_6H_6	-102.7
7	$C_8H_6N_2O_2$ (phthalhydrazide) + CH_3CH_3 → $C_4H_6N_2O_2$ (5,6-dihydrouracil) + C_6H_6	-100.8
8	$C_8H_6N_2O_2$ (phthalhydrazide) + 2 $H_2C{=}CH_2$ → $C_6H_8N_2$ (5,6-dimethyluracil) + C_6H_6	-98.4
9	$C_8H_6N_2O_2$ (phthalhydrazide) + 2 CH_3CH_3 → $C_5H_7NO_2$ (glutarimide) + C_6H_6 + CH_3NH_2	-99.4
10	$C_8H_6N_2O_2$ (phthalhydrazide) + CH_3CH_3 → $C_7H_6N_2O$ (3-indazolinone) + $CH_3C(O)CH_3$	-99.6
11	$C_8H_6N_2O_2$ (phthalhydrazide) + CH_3CH_3 → $C_7H_6N_2O$ (2-benzimidazolinone) + $CH_3C(O)CH_3$	-95.8
	average of 11 reactions	**-98.8**

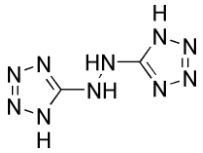
1-hydrazinyl-2,2-dinitroethenamine, H-FOX: $(O_2N)_2C{=}C(NH_2)(NHNH_2)$ (33)

atomization reaction		106.0
reactions with FOX-7: $(O_2N)_2C{=}C(NH_2)_2$		
1	$(O_2N)_2C{=}C(NH_2)(NHNH_2)$ + CH_3CH_3 → $(O_2N)_2C{=}C(NH_2)_2$ + CH_3NHCH_3	111.1
2	$(O_2N)_2C{=}C(NH_2)(NHNH_2)$ + CH_4 → $(O_2N)_2C{=}C(NH_2)_2$ + CH_3NH_2	109.3
3	$(O_2N)_2C{=}C(NH_2)(NHNH_2)$ + H_2O → $(O_2N)_2C{=}C(NH_2)_2$ + NH_2OH	110.6
4	$(O_2N)_2C{=}C(NH_2)(NHNH_2)$ + HC(O)H → $(O_2N)_2C{=}C(NH_2)_2$ + $HC(O)NH_2$	108.2
5	$(O_2N)_2C{=}C(NH_2)(NHNH_2)$ + CH_3NHCH_3 → $(O_2N)_2C{=}C(NH_2)_2$ + HN=NH + CH_3CH_3	108.4
6	$(O_2N)_2C{=}C(NH_2)(NHNH_2)$ + CH_3NH_2 → $(O_2N)_2C{=}C(NH_2)_2$ + CH_3NHNH_2	110.9
7	$(O_2N)_2C{=}C(NH_2)(NHNH_2)$ + CH_3NHCH_3 → $(O_2N)_2C{=}C(NH_2)_2$ + $(CH_3)_2NNH_2$	
	average of 7 reactions (1-7) with FOX-7	**110.1**
reactions with different species		
8	$(O_2N)_2C{=}C(NH_2)(NHNH_2)$ + 2 •CH_3 + 3 •H → $H_2C{=}C(CH_3)_2$ + 2 •NO_2 + 3 •NH_2	111.1
9	$(O_2N)_2C{=}C(NH_2)(NHNH_2)$ + 2 •CH_3 + 3 •H → $CH_3CH{=}CHCH_3$ + 2 •NO_2 + 3 •NH_2	111.1
10	$(O_2N)_2C{=}C(NH_2)(NHNH_2)$ + 3 •CH_3 + 2 •H → $CH_3CH{=}C(CH_3)_2$ + 2 •NO_2 + 3 •NH_2	109.4
11	$(O_2N)_2C{=}C(NH_2)(NHNH_2)$ + 2 CH_4 → $H_2C{=}C(CH_3)_2$ + O_2NNO_2 + NH_3 + NH=NH	107.2
12	$(O_2N)_2C{=}C(NH_2)(NHNH_2)$ + 2 CH_3CH_3 + 3 CH_4 → $H_2C{=}C(CH_3)_2$ + 3 CH_3NH_2 + 2 CH_3NO_2	114.8
13	$(O_2N)_2C{=}C(NH_2)(NHNH_2)$ + 5 CH_4 → 2 CH_3NO_2 + 3 CH_3NH_2 + $H_2C{=}CH_2$	115.3
14	$(O_2N)_2C{=}C(NH_2)(NHNH_2)$ + 2 CH_4 → O_2NNO_2 + H_2NNH_2 + NH_3 + $H_2C{=}CH{-}CH{=}CH_2$	101.8
15	$(O_2N)_2C{=}C(NH_2)(NHNH_2)$ → 2 HNO_2 + HN_3 + HC≡CH	102.9
16	$(O_2N)_2C{=}C(NH_2)(NHNH_2)$ + 7 CH_4 → 2 HNO_2 + CH_3NHNH_2 + CH_3NHCH_3 + 3 CH_3CH_3	106.6
17	$(O_2N)_2C{=}C(NH_2)(NHNH_2)$ + 5 CH_4 → O_2NNO_2 + CH_3NHNH_2 + CH_3NHCH_3 + 2 CH_3CH_3	113.7
18	$(O_2N)_2C{=}C(NH_2)(NHNH_2)$ + 7 CH_4 → 2 HNO_2 + $(CH_3)_2NNH_2$ + CH_3NH_2 + 3 CH_3CH_3	106.4
19	$(O_2N)_2C{=}C(NH_2)(NHNH_2)$ + 5 CH_4 → O_2NNO_2 + $(CH_3)_2NNH_2$ + CH_3NH_2 + 2 CH_3CH_3	113.5
20	$(O_2N)_2C{=}C(NH_2)(NHNH_2)$ + 4 CH_4 → 2 CH_3NHNO_2 + CH_3NHCH_3 + CH_3CH_3	118.2
21	$(O_2N)_2C{=}C(NH_2)(NHNH_2)$ + 3 CH_4 → 2 $CH_3N(NO_2)CH_3$ + CH_3NH_2	115.7
	average of 14 reactions (8-21) with different species	**110.6**
	average of all 21 reactions	**110.4**

3,6-dihydrazino-1,2,4,5-tetrazine, DHT:  **(34)**

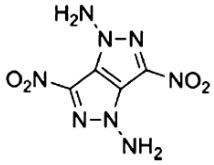
atomization reaction		663.3
reactions with different species		
1	$C_2H_6N_8$ (DHT) + 2 CH_4 → $C_2H_2N_4$ (1,2,4,5-tetrazine) + 2 CH_3NHNH_2	660.1
2	$C_2H_6N_8$ (DHT) + 2 CH_3CH_3 → $C_2H_2N_4$ (1,2,4,5-tetrazine) + 2 $(CH_3)_2NNH_2$	663.6
3	$C_2H_6N_8$ (DHT) → $C_2H_2N_4$ (1,2,4,5-tetrazine) + 2 HN=NH	658.3
4	$C_2H_6N_8$ (DHT) + 2 CH_4 + C_6H_6 → 2 $C_4H_4N_2$ (pyridazine) + 2 CH_3NHNH_2	664.4

5	$C_2H_6N_8$ (DHT) + 2 CH_3CH_3 + C_6H_6 → 2 $C_4H_4N_2$ (pyridazine) + 2 $(CH_3)_2NNH_2$	667.9
6	$C_2H_6N_8$ (DHT) + C_6H_6 → 2 $C_4H_4N_2$ (pyridazine) + 2 HN=NH	662.6
7	$C_2H_6N_8$ (DHT) + 2 CH_4 + C_6H_6 → 2 $C_4H_4N_2$ (pyrimidine) + 2 CH_3NHNH_2	669.4
8	$C_2H_6N_8$ (DHT) + 2 CH_3CH_3 + C_6H_6 → 2 $C_4H_4N_2$ (pyrimidine) + 2 $(CH_3)_2NNH_2$	672.9
9	$C_2H_6N_8$ (DHT) + C_6H_6 → 2 $C_4H_4N_2$ (pyrimidine) + 2 HN=NH	667.7
10	$C_2H_6N_8$ (DHT) + 2 CH_4 + C_6H_6 → $C_4H_4N_2$ (pyridazine) + $C_4H_4N_2$ (pyrimidine) + 2 CH_3NHNH_2	667.3
11	$C_2H_6N_8$ (DHT) + 2 CH_3CH_3 + C_6H_6 → $C_4H_4N_2$ (pyridazine) + $C_4H_4N_2$ (pyrimidine) + 2 $(CH_3)_2NNH_2$	670.4
12	$C_2H_6N_8$ (DHT)+ C_6H_6 → $C_4H_4N_2$ (pyridazine) + $C_4H_4N_2$ (pyrimidine) + 2 HN=NH	665.1
13	$C_2H_6N_8$ (DHT) + 6 CH_4 → 4 HN=NH + $H_2C=CH_2$ + 3 CH_3CH_3	658.7
	average of 13 reactions	**665.3**

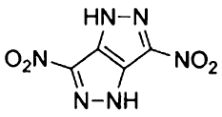
5,5'-hydrazinebistetrazole, HBT:  **(35)**

atomization reaction		810.7
reactions with 1H-tetrazole		
1	$C_2H_4N_{10}$ (HBT) + 2 CH_4 → 2 CH_2N_4 (1*H*-tetrazole) + HN=NH + CH_3CH_3	802.6
2	$C_2H_4N_{10}$ (HBT) + 2 CH_4 → 2 CH_2N_4 (1*H*-tetrazole) + $(CH_3)_2NNH_2$	805.2
3	$C_2H_4N_{10}$ (HBT) + 3 CH_4 → 2 CH_2N_4 (1*H*-tetrazole) + CH_3NHNH_2 + CH_3CH_3	803.6
4	$C_2H_4N_{10}$ (HBT) + C_4H_4O (furan) + HC(O)H → 2 CH_2N_4 (1*H*-tetrazole) + $C_5H_6N_2O_2$ [2-fur-C(O)$NHNH_2$]	805.8
5	$C_2H_4N_{10}$ (HBT) + $C_6H_5CH_3$ + 2 CH_4 → 2 CH_2N_4 (1*H*-tetrazole) + $C_6H_5N(CH_3)NH_2$ + CH_3CH_3	807.6
	average of 5 reactions (1-5) with 1*H*-tetrazole	**804.9**
reactions with 5-methyl-1H-tetrazole		
6	$C_2H_4N_{10}$ (HBT) + CH_3CH_3 → 2 $C_2H_4N_4$ (5-methyl-1*H*-tetrazole) + HN=NH	804.8
7	$C_2H_4N_{10}$ (HBT) + 2 CH_3CH_3 → 2 $C_2H_4N_4$ (5-methyl-1*H*-tetrazole) + $(CH_3)_2NNH_2$	807.5
8	$C_2H_4N_{10}$ (HBT) + CH_4 + CH_3CH_3 → 2 $C_2H_4N_4$ (5-methyl-1*H*-tetrazole) + CH_3NHNH_2	805.8
9	$C_2H_4N_{10}$ (HBT) + C_4H_4O (furan) + $CH_3C(O)CH_3$ → 2 $C_2H_4N_4$ (5-methyl-1*H*-tetrazole) + $C_5H_6N_2O_2$ [2-fur-C(O)$NHNH_2$]	809.8
10	$C_2H_4N_{10}$ (HBT) + $C_6H_5CH_3$ + CH_3CH_3 → 2 $C_2H_4N_4$ (5-methyl-1*H*-tetrazole) + $C_6H_5N(CH_3)NH_2$	809.9
	average of 5 reactions (6-10) with 5-methyl-1*H*-tetrazole	**807.6**
reactions with 5-amino-1H-tetrazole		
11	$C_2H_4N_{10}$ (HBT) + 2 CH_4 → 2 CH_3N_5 (5-amino-1*H*-tetrazole) + CH_3CH_3	806.3
12	$C_2H_4N_{10}$ (HBT) + CH_3CH_3 → 2 CH_3N_5 (5-amino-1*H*-tetrazole) + $H_2C=CH_2$	805.3
13	$C_2H_4N_{10}$ (HBT) + $CH_3CH(OH)CH_3$ → 2 CH_3N_5 (5-amino-1*H*-tetrazole) + $CH_3C(O)CH_3$	805.1
	average of 3 reactions (11-13) with 5-amino-1*H*-tetrazole	**805.6**
reaction with 1-methyl-5-amino-1H-tetrazole		
14	$C_2H_4N_{10}$ (HBT) + CH_3CH_3 → 2 $C_2H_5N_5$ (1-methyl-5-amino-1*H*-tetrazole)	**806.0**
reactions with 5-phenyl-1H-tetrazole		
15	$C_2H_4N_{10}$ (HBT) + 2 $C_6H_5CH_3$ → 2 $C_7H_6N_4$ (5-phenyl-1*H*-tetrazole) + $(CH_3)_2NNH_2$	808.2
16	$C_2H_4N_{10}$ (HBT) + C_6H_6 + $C_6H_5CH_3$ → 2 $C_7H_6N_4$ (5-phenyl-1*H*-tetrazole) + CH_3NHNH_2	807.7
	average of 2 reactions (15-16) with 5-phenyl-1*H*-tetrazole	**808.0**
reactions with two different tetrazoles		
17	$C_2H_4N_{10}$ (HBT) + CH_3CH_3 + CH_4 → $C_2H_4N_4$ (5-methyl-1*H*-tetrazole) + CH_2N_4 (1*H*-tetrazole) + $(CH_3)_2NNH_2$	806.3
18	$C_2H_4N_{10}$ (HBT) + CH_3CH_3 + CH_4	

	→ $C_2H_4N_4$ (5-methyl-1*H*-tetrazole) + CH_2N_4 (1*H*-tetrazole) + $NH_2CH_2CH_2NH_2$	803.7
19	$C_2H_4N_{10}$ (HBT) + 2 CH_4	
	→ $C_2H_4N_4$ (5-methyl-1*H*-tetrazole) + CH_2N_4 (1*H*-tetrazole) + CH_3NHNH_2	804.7
20	$C_2H_4N_{10}$ (HBT) + NH_3 → CH_3N_5 (5-amino-1*H*-tetrazole) + CH_2N_4 (1*H*-tetrazole) + HN=NH	806.9
21	$C_2H_4N_{10}$ (HBT) + NH_3 + CH_4	
	→ CH_3N_5 (5-amino-1*H*-tetrazole) + CH_2N_4 (1*H*-tetrazole) + CH_3NHNH_2	807.9
22	$C_2H_4N_{10}$ (HBT) + CH_3NH_2 + CH_4	
	→ CH_3N_5 (5-amino-1*H*-tetrazole) + CH_2N_4 (1*H*-tetrazole) + $(CH_3)_2NNH_2$	807.3
23	$C_2H_4N_{10}$ (HBT) + 2 CH_4	
	→ $C_2H_4N_4$ (5-methyl-1*H*-tetrazole) + CH_3N_5 (5-amino-1*H*-tetrazole) + CH_3NH_2	805.3
24	$C_2H_4N_{10}$ (HBT) + CH_4 + CH_3CH_3	
	→ $C_2H_4N_4$ (5-methyl-1*H*-tetrazole) + CH_3N_5 (5-amino-1*H*-tetrazole) + CH_3NHCH_3	807.0
25	$C_2H_4N_{10}$ (HBT) + CH_3CH_3	
	→ $C_2H_4N_4$ (5-methyl-1*H*-tetrazole) + CH_3N_5 (5-amino-1*H*-tetrazole) + H_2C=NH	806.0
26	$C_2H_4N_{10}$ (HBT) + CH_4 + H_2O	
	→ $C_2H_5N_5$ (1-methyl-5-amino-1*H*-tetrazole) + CH_2N_4 (1*H*-tetrazole) + NH_2OH	805.0
27	$C_2H_4N_{10}$ (HBT) + CH_4 + CH_3CH_3	
	→ $C_2H_5N_5$ (1-methyl-5-amino-1*H*-tetrazole) + $C_2H_4N_4$ (5-methyl-1*H*-tetrazole) + CH_3NH_2	805.1
28	$C_2H_4N_{10}$ (HBT) + $CH_3CH_2CH_3$	
	→ $C_2H_5N_5$ (1-methyl-5-amino-1*H*-tetrazole) + $C_2H_4N_4$ (5-methyl-1*H*-tetrazole) + H_2C=NH	805.9
29	$C_2H_4N_{10}$ (HBT) + CH_4 + CH_3CN	
	→ $C_2H_5N_5$ (1-methyl-5-amino-1*H*-tetrazole) + $C_2H_4N_4$ (5-methyl-1*H*-tetrazole) + H_2N=CN	804.2
30	$C_2H_4N_{10}$ (HBT) + CH_4 → $C_2H_5N_5$ (1-methyl-5-amino-1*H*-tetrazole) + CH_3N_5 (5-amino-1*H*-tetrazole)	806.1
31	$C_2H_4N_{10}$ (HBT) + C_6H_6 + CH_4	
	→ $C_7H_6N_4$ (5-phenyl-1*H*-tetrazole) + CH_2N_4 (1*H*-tetrazole) + CH_3NHNH_2	806.2
32	$C_2H_4N_{10}$ (HBT) + $C_6H_5CH_3$ + CH_4	
	→ $C_7H_6N_4$ (5-phenyl-1*H*-tetrazole) + CH_2N_4 (1*H*-tetrazole) + $(CH_3)_2NNH_2$	806.7
33	$C_2H_4N_{10}$ (HBT) + $C_6H_5CH_3$	
	→ $C_7H_6N_4$ (5-phenyl-1*H*-tetrazole) + $C_2H_4N_4$ (5-methyl-1*H*-tetrazole) + HN=NH	805.2
34	$C_2H_4N_{10}$ (HBT) + $C_6H_5NH_2$	
	→ $C_7H_6N_4$ (5-phenyl-1*H*-tetrazole) + CH_3N_5 (5-amino-1*H*-tetrazole) + HN=NH	806.0
35	$C_2H_4N_{10}$ (HBT) + CH_3CH_3 + $C_6H_5NH_2$	
	→ $C_7H_6N_4$ (5-phenyl-1*H*-tetrazole) + CH_3N_5 (5-amino-1*H*-tetrazole) + $(CH_3)_2NNH_2$	808.6
36	$C_2H_4N_{10}$ (HBT) + $C_6H_5CH_3$ + CH_4	
	→ $C_7H_6N_4$ (5-phenyl-1*H*-tetrazole) + CH_3N_5 (5-amino-1*H*-tetrazole) + CH_3NHCH_3	807.5
37	$C_2H_4N_{10}$ (HBT) + C_6H_6 + H_2O	
	→ $C_7H_6N_4$ (5-phenyl-1*H*-tetrazole) + CH_3N_5 (5-amino-1*H*-tetrazole) + NH_2OH	807.8
38	$C_2H_4N_{10}$ (HBT) + $C_6H_5CH_2NH_2$ + CH_4	
	→ $C_7H_6N_4$ (5-phenyl-1*H*-tetrazole) + $C_2H_5N_5$ (1-methyl-5-amino-1*H*-tetrazole) + CH_3NHNH_2	806.7
	average of 22 reactions (17-38) with two different tetrazoles	**806.2**
	average of all 38 reactions	**806.3**

1,4-diamino-3,6-dinitropyrazolo[4,3-c]pyrazole, DADNP, LLM-119:  **(36)**

atomization reaction 611.3

reactions with DNPP: 

1	$C_4H_4N_8O_4$ (DADNP) → $C_4H_2N_6O_4$ (DNPP) + HN=NH	625.5
2	$C_4H_4N_8O_4$ (DADNP) + CH_3CH_3 → $C_4H_2N_6O_4$ (DNPP) + 2 CH_3NHCH_3	628.5
3	$C_4H_4N_8O_4$ (DADNP) + CH_4 → $C_4H_2N_6O_4$ (DNPP) + CH_3NHNH_2	626.5
4	$C_4H_4N_8O_4$ (DADNP) + CH_3CH_3 → $C_4H_2N_6O_4$ (DNPP) + $(CH_3)_2NNH_2$	628.1

	average of 4 reactions with DNPP	**627.2**
reactions with different species		
5	$C_4H_4N_8O_4$ (DADNP) + 12 CH_4 → 3 HN=NH + 2 CH_3NO_2 + $H_2C{=}CH_2$ + 6 CH_3CH_3	624.5
6	$C_4H_4N_8O_4$ (DADNP) + 2 CH_3CH_3 → 2 $C_3H_4N_2$ (1*H*-pyrazole) + 2 CH_3NO_2 + HN=NH	627.1
7	$C_4H_4N_8O_4$ (DADNP) + 2 $CH_3CH_2CH_3$ → 2 $C_3H_4N_2$ (1*H*-pyrazole) + 2 $CH_3CH_2NO_2$ + HN=NH	625.6
8	$C_4H_4N_8O_4$ (DADNP) + 2 CH_3CH_3 → 2 $C_3H_4N_2$ (1*H*-imidazole) + 2 CH_3NO_2 + HN=NH	625.9
9	$C_4H_4N_8O_4$ (DADNP) + 2 C_6H_6 + 4 CH_4 → 2 $C_7H_6N_2$ (1*H*-indazole) + 2 CH_3NO_2 + 2 CH_3CH_3 + HN=NH	623.7
	average of 5 reactions with different species	**625.4**
	average of all 9 reactions	**626.2**

[a]Experimental enthalpies of formation of reference species used in isodesmic reactions were taken from ATcT (black marked species), Table S1 (blue marked species), and Table 2 (hydrazines, green marked species). The values recommended from isodesmic reaction calculations are given in red. [b]Enthalpy formation values for this compound were calculated from G4MP2 energies.

Table S3. Molecular Electrostatic Potential Parameters Calculated for the Molecular Geometries Optimized at the B3LYP/cc-pVTZ Level, Regression Coefficients *a*, *b*, *c*, and *d* for Enthalpies of Sublimation and Vaporization, and Comparison Between Experimental and Calculated Enthalpies of Sublimation and Vaporization

crystal compounds

$$\Delta_{sub}H^{\circ}_{298} = a(SA)^2 + b\sqrt{\sigma^2_{tot}\upsilon} + c + d\Pi$$

$a = 0.0003163$ kcal/mol×Å^{-4}, $b = 1.3345230$, $c = 0.7774774$ kcal/mol, $d = -4.4267916$

compound[a]		$\Delta_{sub}H^{\circ}_{298}$ kJ/mol exp	$\Delta_{sub}H^{\circ}_{298}$ kJ/mol calc	exp – calc	(SA), A^2	σ^2_{tot}, (kcal/mol)^2	υ	Π, kcal/mol
			calibration set of compounds					
CH_4N_2S	$H_2NC(S)NH_2$	112.0	111.5	0.5	109.80665	267.8164764	0.2111478	22.1639933
CH_5N_3O	$H_2NN(CH_3)NO$ (**9**)	79.5	88.2	-8.7	111.12282	171.6457015	0.23933415	16.77313848
CH_5N_3S	$H_2NC(S)NHNH_2$ (**26**)	125.8	117.3	8.5	124.90551	251.1175632	0.24340575	21.98317439
$C_2H_3N_3$	1*H*-1,2,4-triazole	84.0	95.8	-11.8	99.17951	300.1044715	0.22180828	17.12347663
$C_2H_4N_2O_2$	$H_2NC(O)C(O)NH_2$	117.3	99.7	17.6	115.70322	264.6323229	0.24635362	17.0389701
$C_2H_4N_4O_4$	$(O_2N)_2C{=}C(NH2)_2$ (FOX-7)	122.6	135.0	-12.4	151.70926	396.9328007	0.18264774	23.22863224
$C_2H_5N_3O_2$	$H_2NC(O)NHC(O)NH_2$	126.7	118.7	8.0	130.26551	364.2907406	0.24151745	19.1713514
$C_2H_6N_2O$	$NH_2C(O)NHCH_3$	95.9	103.5	-7.6	115.93276	332.3652367	0.23571098	16.84051582
$C_3H_3N_3$	1,3,5-triazine	54.2	57.8	-3.6	111.06101	81.2128326	0.22095002	11.1731431
$C_3H_4N_2$	1*H*-pyrazole	74.0	81.8	-7.8	104.45961	214.1721246	0.2436117	14.0143712
$C_3H_6N_2O$	imidazolidin-2-one	96.6	94.1	2.5	121.69918	248.5637267	0.14609221	18.26384629
$C_3H_8N_2O$	$NH_2C(O)NHCH_2CH_3$	99.3	102.3	-3.0	136.82741	333.2319446	0.23289306	14.4022103
$C_3H_8N_2O$	$H_2NC(O)N(CH_3)_2$	93.5	93.1	0.4	133.62748	274.0916771	0.17098075	15.3074111
$C_4H_4N_2$	pyrazine	57.5	60.5	-3.0	116.28031	115.5875181	0.21472613	10.24808999
$C_4H_6N_2O_2$	5,6-dihydrouracil	115.4	106.3	9.1	141.75666	192.8361577	0.24080758	18.49687021
$C_4H_{10}N_2O$	$NH_2C(O)NHCH(CH_3)_2$	98.1	102.3	-4.2	155.96472	314.3357348	0.2207068	12.96359665
$C_5H_6N_2$	2-aminopyridine	78.7	76.9	1.8	135.68106	136.0975556	0.24900119	11.83867754
$C_5H_6N_2O_2$	2-furancarboxylic acid hydrazide (**28**)	99.0	91.1	7.9	158.42564	209.2964213	0.20830586	12.1513137
$C_5H_7NO_2$	glutarimide	86.1	92.2	-6.1	146.73672	130.0883717	0.20447011	16.42777279
C_5H_8N2	3,5-dimethylpyrazole	83.4	83.6	-0.2	149.26037	175.7563052	0.24285095	11.11990898
$C_5H_{11}NO$	$(CH_3)_3CC(O)NH_2$	86.6	93.3	-6.7	153.63028	288.7729562	0.19315268	11.9485506
$C_5H_{12}N_2O$	$CH_3CH_2NHC(O)NHCH_2CH_3$	97.1	102.9	-5.8	179.04685	275.8507576	0.22243729	10.83788095
$C_6H_6N_2O$	2-pyridinecarboxamide	93.1	92.1	1.0	156.3396	230.9124448	0.19490639	12.54381801
$C_6H_6N_2O_2$	2-nitroaniline	89.0	100.0	-11.0	162.07443	230.0439509	0.24789725	12.77597216
$C_6H_9N_3$	2-amino-4,6-dimethylpyrimidine	89.3	81.5	7.8	173.11876	114.3028745	0.24145405	9.53528969

$C_6H_9N_3$	4-amino-2,6-dimethylpyrimidine	99.6	93.7	5.9	173.41873	189.0021044	0.24495884	10.59336674
$C_7H_6N_2$	1*H*-indazole	91.1	82.3	8.8	154.15097	145.5726391	0.23872405	11.2115931
$C_7H_6N_2O$	3-indazolinone (**31**)	127.6	108.5	19.1	163.40255	283.8468003	0.23619877	14.1347959
$C_7H_6N_4$	5-phenyl-1*H*-tetrazole	115.0	122.5	-7.5	176.87092	314.3686137	0.24914547	15.43215157
C_7H_7NO	$C_6H_5C(O)NH_2$	103.1	100.3	2.8	160.76551	240.7713781	0.23218237	13.16857719
$C_7H_8N_2O$	2-aminobenzamide	106.8	97.8	9.0	170.89502	165.5969939	0.24864975	12.87157009
C_7H_9N	1,4-H_2N-C_6H_4-CH_3	76.2	76.2	0.0	161.21919	116.4909874	0.24419187	9.40142811
C_8H_9NO	$C_6H_5NHC(O)CH_3$	100.3	103.3	-3.0	183.06308	180.6510064	0.24583331	12.37741983
$C_{12}H_{10}N_2$	$C_6H_5N{=}NC_6H_5$	94.1	95.8	-1.7	233.90759	33.5980829	0.24881216	7.91267276
$C_{12}H_{11}N$	$C_6H_5NHC_6H_5$	95.2	95.0	0.2	220.82249	66.9151718	0.21699964	8.52117383
$C_{13}H_{11}N$	$C_6H_5CH{=}NC_6H_5$	98.1	103.1	-5.0	238.42576	49.1337858	0.24212396	8.35327838
			root-mean-square deviation	7.6				
			hydrazine derivatives					
CH_5N_3O	$H_2NC(O)NHNH_2$ (**19**)		111.6		109.25804	350.8516751	0.21238378	20.31535412
CH_6N_4O	$H_2NNHC(O)NHNH_2$ (**20**)		107.4		124.91065	302.4379757	0.23900381	17.75638185
CH_6N_4S	$H_2NNHC(S)NHNH_2$ (**27**)	152.1	108.0		138.8304	237.7042423	0.22559987	18.4739379
$C_2H_4N_2O_2$	HC(O)NHNHC(O)H (**21**)	100.8 205.1	98.9		118.98391	206.6722301	0.2460889	18.09175332
$C_2H_4N_{10}$	5,5'-hydrazinebistetrazole (**35**)		149.3		181.95146	363.9350379	0.16436035	24.85640332
$C_2H_5N_5O_4$	$(O_2N)2C{=}C(NH_2)(NHNH_2)$ (**33**)		140.2		166.52428	307.3737705	0.2286754	23.13394263
$C_2H_6N_4O_2$	$H_2NC(O)NHNHC(O)NH_2$ (**24**)		123.2		147.67732	286.1858869	0.24853683	20.20765572
$C_2H_6N_4O_2$	$H_2NNHC(O)C(O)NHNH_2$ (**25**)		91.9		147.72839	144.6830625	0.24991748	14.75694763
$C_2H_6N_8$	3,6-dihydrazino-1,2,4,5-tetrazine (**34**)		94.0		167.14626	132.8001253	0.24884761	13.34880455
$C_2H_8N_6O_2$	$H_2NN(NO)CH_2CH_2N(NO)NH_2$ (**10**)	172.4	106.8		173.46887	138.8758625	0.24925388	16.19093343
$C_4H_4N_8O_4$	1,4-diamino-3,6-dinitropyrazolo[4,3-c]-pyrazole (**36**)		130.9		212.64024	182.2555485	0.19796726	17.22459314
$C_4H_8N_2O_2$	$CH_3C(O)NHNHC(O)CH_3$ (**22**)	103.1	97.3		162.25404	171.2864941	0.21784294	14.39595862
$C_6H_7N_3O$	4-pyridinecarboxylic acid hydrazide (**29**)	101.0	100.1		171.86601	189.1721437	0.24608843	12.73911115
$C_6H_7N_3O_2$	2-nitrophenylhydrazine (**17**)	124.7	105.4		177.04983	222.3377305	0.24988722	12.55751747
$C_7H_8N_2O$	benzoic acid hydrazide (**30**)		94.8		176.19166	173.7464703	0.21910419	11.60880068
$C_8H_6N_2O_2$	phthalhydrazide (**32**)	139.8	118.3		180.03359	298.3246267	0.24941881	14.07241391
$C_{12}H_{10}N_4O_4$	4,4'-O_2N-C_6H_4-NHNH-C_6H_4-NO_2 (**18**)		181.4		288.37867	223.4274739	0.22697303	15.4141248
$C_{12}H_{12}N_2$	$C_6H_5NHNHC_6H_5$ (**13**)		108.8		236.30832	80.4079354	0.21789872	9.2272378
$C_{12}H_{12}N_2$	$(C_6H_5)_2NNH_2$ (**14**)		103.2		231.09517	76.5482423	0.22129957	8.61393496
$C_{14}H_{12}N_2O_2$	$C_6H_5C(O)NHNHC(O)C_6H_5$ (**23**)		147.7		281.55762	130.7464784	0.20124864	10.05393412
$C_{18}H_{16}N_2$	$(C_6H_5)_2NNHC_6H_5$ (**15**)		153.4		309.95151	50.9512606	0.24328142	7.73469645
$C_{24}H_{20}N_2$	$(C_6H_5)_2NN(C_6H_5)_2$ (**16**)		206.1		373.50771	37.2039049	0.21254978	7.46716453

liquid compounds

$$\Delta_{vap}H^{\circ}_{298} = a(SA)^2 + b\sqrt{\sigma^2_{tot}\upsilon} + c + d\Pi$$

$a = 0.0003314$ kcal/mol×Å^{-4}, $b = -1.0589324$, $c = 0.6697609$ kcal/mol, $d = 3.7598004$

compound		$\Delta_{vap}H^{\circ}_{298}$ kJ/mol exp	$\Delta_{vap}H^{\circ}_{298}$ kJ/mol calc	exp – calc	(SA), A^2	σ^2_{tot}, (kcal/mol)^2	υ	Π, kcal/mol
			calibration set of compounds					
CH_6N_2	CH_3NHNH_2 (**1**)	40.4	41.4	-1.0	93.85926	129.9522837	0.16836400	11.82364256
$C_2H_8N_2$	$(CH_3)_2NNH_2$ (**2**)	35.0	36.3	-1.3	113.30302	140.9585147	0.19450847	8.82293581
$C_2H_8N_2$	$CH_3NHNHCH_3$ (**3**)	39.3	36.6	2.7	115.26147	122.8661947	0.16695816	9.07123403
$C_3H_{10}N_2$	$(CH_3)_2NNH(CH_3)$ (**5**)	33.3	33.3	0.0	134.59847	94.6070747	0.13937359	6.91102467
$C_4H_{12}N_2$	$(CH_3)_2NN(CH_3)_2$ (**7**)	32.9	33.7	-0.8	147.78410	95.5300995	0.09536344	5.88274815
$C_7H_{10}N_2$	$C_6H_5N(CH_3)NH_2$ (**12**)	63.2	62.9	0.3	172.01488	73.3935272	0.24844708	9.01177795
		root-mean-square deviation		1.3				
			hydrazine derivatives					
$C_2H_8N_2$	$CH_3CH_2NHNH_2$ (**4**)		40.0		115.67896	139.8930053	0.16074432	9.71429498
$C_3H_{10}N_2$	$(CH_3)_2CHNHNH_2$ (**6**)		42.0		132.79444	149.6056593	0.1563457	8.49725144
$C_4H_{12}N_2$	$(CH_3)_3CNHNH_2$ (**8**)		47.6		147.91466	107.5099869	0.24881438	7.98323211
$C_6H_8N_2$	$C_6H_5NHNH_2$ (**11**)	61.9	61.4	0.5	154.42504	92.51479180	0.23727894	10.65517901

[a]Hydrazines are marked in green; the compound's number according to Table 2 is given for each molecule.