


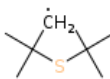

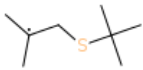
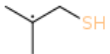



## RMG Output

### Species (51)

Index	Thermo H298 (kcal/mol), S298 (cal/mol*K), Cp (cal/mol*K)						Structure	Label	SMILES	MW (g/mol)
-1.	<b>H298</b>	<b>S298</b>	<b>Cp300</b>	<b>Cp500</b>	<b>Cp1000</b>	<b>Cp1500</b>	Ar	Ar	[Ar]	39.35
	-0.00	37.01	4.97	4.97	4.97	4.97				
-1.	<b>H298</b>	<b>S298</b>	<b>Cp300</b>	<b>Cp500</b>	<b>Cp1000</b>	<b>Cp1500</b>	He	He	[He]	4.00
	-0.00	30.15	4.97	4.97	4.97	4.97				
-1.	<b>H298</b>	<b>S298</b>	<b>Cp300</b>	<b>Cp500</b>	<b>Cp1000</b>	<b>Cp1500</b>	Ne	Ne	[Ne]	20.18
	-0.00	34.97	4.97	4.97	4.97	4.97				
-1.	<b>H298</b>	<b>S298</b>	<b>Cp300</b>	<b>Cp500</b>	<b>Cp1000</b>	<b>Cp1500</b>	$\text{N}\equiv\text{N}$	N2	N#N	28.01
	-0.00	45.79	6.96	7.07	7.81	8.31				
1.	<b>H298</b>	<b>S298</b>	<b>Cp300</b>	<b>Cp500</b>	<b>Cp1000</b>	<b>Cp1500</b>		DTBS(1)	CC(C)(C)SC(C)(C)C	146.29
	-45.07	106.76	52.54	77.08	110.96	126.50				
2.	<b>H298</b>	<b>S298</b>	<b>Cp300</b>	<b>Cp500</b>	<b>Cp1000</b>	<b>Cp1500</b>	H <sub>2</sub> S	H2S(2)	S	34.08
	-4.90	49.18	8.18	8.88	10.93	12.29				
3.	<b>H298</b>	<b>S298</b>	<b>Cp300</b>	<b>Cp500</b>	<b>Cp1000</b>	<b>Cp1500</b>		C4H8(3)	C=C(C)C	56.11
	-3.80	69.99	21.54	31.20	46.91	54.64				
4.	<b>H298</b>	<b>S298</b>	<b>Cp300</b>	<b>Cp500</b>	<b>Cp1000</b>	<b>Cp1500</b>		C4H9SH(4)	CC(C)(C)S	90.19
	-25.99	83.68	30.57	42.84	59.68	68.12				
5.	<b>H298</b>	<b>S298</b>	<b>Cp300</b>	<b>Cp500</b>	<b>Cp1000</b>	<b>Cp1500</b>		C4H10(5)	CC(C)C	58.12
	-32.50	70.43	23.06	35.25	54.22	63.87				
6.	<b>H298</b>	<b>S298</b>	<b>Cp300</b>	<b>Cp500</b>	<b>Cp1000</b>	<b>Cp1500</b>		C6H10(6)	C1=CCCCC1	82.14
	-1.03	74.20	24.44	41.15	65.49	76.90				
7.	<b>H298</b>	<b>S298</b>	<b>Cp300</b>	<b>Cp500</b>	<b>Cp1000</b>	<b>Cp1500</b>	S=S	S2(7)	S=S	64.13
	47.12	53.78	7.82	8.39	8.75	8.88				

8.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b>	$\cdot\text{S}-\text{S}\cdot$	S2JJ(8)	[S][S]	64.13
	30.74 54.54 7.80 8.35 8.91 9.32				
9.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b>		C4H8JSH(9)	[CH2]C(C)(C)S	89.18
	23.01 89.28 29.76 40.99 55.88 63.48				
10.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b>		C4H9SJ(10)	CC(C)(C)[S]	89.18
	9.73 80.98 27.32 39.29 56.37 64.66				
11.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b>	$\cdot\text{HS}$	HSJ(11)	[SH]	33.07
	33.30 46.76 7.74 7.50 7.90 8.33				
12.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b>	$\text{HS}-\text{SH}$	HSSH(12)	SS	66.15
	3.40 60.38 11.88 14.19 16.80 17.86				
15.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b>		C4H9(15)	C[C](C)C	57.11
	11.90 74.29 22.20 31.86 49.45 58.50				
18.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b>		C8H17S(18)	[CH2]C(C)(C)SC(C)(C)C	145.29
	3.93 113.73 51.72 75.24 107.15 121.86				
19.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b>	$\text{H}\cdot$	H(19)	[H]	1.01
	52.10 27.42 4.97 4.97 4.97 4.97				
28.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b>		C4H7(28)	[CH2]C(=C)C	55.10
	32.30 69.61 20.96 30.41 44.29 51.20				
39.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b>		C8H17S(39)	C[C](C)CSC(C)(C)C	145.29
	-2.52 119.94 50.60 72.49 105.21 121.58				
40.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b>		C4H9S(40)	C[C](C)CS	89.18
	21.24 90.84 27.52 37.55 54.89 63.60				
64.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b>		C6H9(64)	[CH]1C=CCCC1	81.14
	30.04 73.79 24.28 39.39 61.84 71.86				
71.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b>		C6H11(71)	[CH]1CCCCC1	83.15

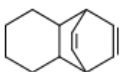
13.90 79.55 25.48 42.63 71.37 83.40



75.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b> 3.22 117.66 54.75 84.93 128.79 146.16		S(75)	CC(C)(C)SC1[CH]CCCC1	171.32
80.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b> 24.85 91.46 31.36 49.66 77.82 88.55		C6H11S(80)	SC1[CH]CCCC1	115.22
99.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b> -10.22 105.00 47.59 77.91 122.63 140.83		C10H19(99)	CC(C)(C)C1[CH]CCCC1	139.26
102.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b> 25.00 72.52 22.69 37.52 58.02 67.54		C6H8(102)	C1C=CCCC=1	80.13
127.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b> 19.42 111.77 44.93 70.84 110.51 128.77		S(127)	C[C](C)CC1C=CCCC1	137.24
132.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b> -3.75 48.82 51.82 78.48 115.93 131.64		S(132)	CC1(C)CC2CCC[CH]C21	137.24
134.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b> 21.04 108.62 47.62 83.17 135.80 156.34		S(134)	[CH]1CCCCC1C1C=CCCC1	163.28
137.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b> -2.44 31.59 60.74 91.31 134.96 153.47		S(137)	[CH]1CCCC2C1C1CCCCC21	163.28
146.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b> 4.50 106.83 46.90 80.36 126.44 147.54		S(146)	C1=CC(CCC1)C1C=CCCC1	162.27
239.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b> 66.13 82.29 25.93 39.91 59.11 69.39		C6H8(239)	[CH2]C=CC=C[CH2]	80.13
241.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b> 48.64 70.60 22.31 35.69 54.42 62.58		C6H7(241)	[CH]1C=CC=CC1	79.12
253.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b> 14.80 108.50 54.90 83.54 119.48 136.64		S(253)	CC(C)(C)SC1C=C[CH]CC1	169.31

254.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b> 28.25 116.75 54.90 82.66 118.44 135.22		S(254)	CC(C)(C)SC1[CH]CCC=C1	169.31
268.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b> -20.47 42.17 49.75 76.81 112.35 127.74		S(268)	CC1(C)CC2C=CC1CC2	136.23
275.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b> -19.16 24.94 58.54 89.71 131.29 149.49		S(275)	C1=CC2CCC1C1CCCCC21	162.27
289.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b> 8.47 22.80 55.15 85.01 123.63 140.51		S(289)	C1=CC2C3C=CC(CC3)C2CC1	160.26
312.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b> 56.01 78.16 24.87 38.33 57.36 66.37		C6H8(312)	C=CC1C=CC1	80.13
316.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b> 39.64 79.36 28.08 41.82 58.08 66.37		C6H8(316)	C=CC=CC=C	80.13
781.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b> 49.97 72.25 17.66 26.89 42.31 50.05		C4H7(781)	C[C]1CC1	55.10
1143.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b> 34.31 7.59 26.10 40.36 58.51 66.46		C6H7(1143)	[CH]1C=CC2CC12	79.12
1146.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b> 19.80 64.36 19.90 33.06 50.07 57.93		C6H6(1146)	C1=CC=CC=C1	78.11
1549.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b> -0.00 31.23 6.92 6.97 7.22 7.72	H <sub>2</sub>	H2(1549)	[H][H]	2.02
1552.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b> -29.50 69.71 27.27 46.47 76.01 88.39		S(1552)	C1CCCCC1	84.16
1594.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b> 7.33 36.59 49.30 72.72 105.06 118.30		S(1594)	CC1(C)CC2C=CC1C=C2	134.22
1598.	<b>H298 S298 Cp300 Cp500 Cp1000 Cp1500</b>		S(1598)	C1=CC2C=CC1C1CCCCC21	160.26

8.64 19.36 57.99 85.70 123.88 140.04



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1601.	<b>H298</b>	<b>S298</b>	<b>Cp300</b>	<b>Cp500</b>	<b>Cp1000</b>	<b>Cp1500</b>		S(1601)	[CH]1C=CC(C=C1)C1C=CCCC1	159.25
	56.29	100.31	42.78	74.10	116.12	135.73				

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1608.	<b>H298</b>	<b>S298</b>	<b>Cp300</b>	<b>Cp500</b>	<b>Cp1000</b>	<b>Cp1500</b>		S(1608)	C1C=CC2C3C=CC(CC3)C2C=1	158.24
	32.14	16.72	53.13	82.02	116.69	132.07				