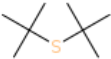
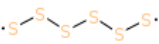
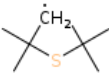
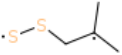
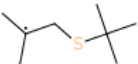
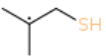
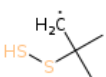
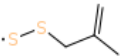
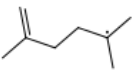
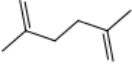
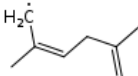
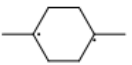


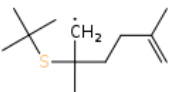
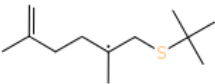
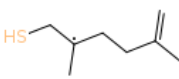
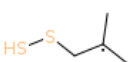
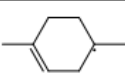
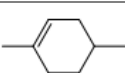
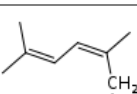
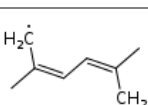
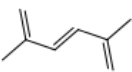
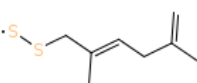
RMG Output

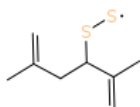
Species (147)

Index	Thermo H298 (kcal/mol), S298 (cal/mol*K), Cp (cal/mol*K)	Structure	Label	SMILES	MW (g/mol)
-1.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 -0.00 37.01 4.97 4.97 4.97 4.97	Ar	Ar	[Ar]	39.35
-1.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 -0.00 30.15 4.97 4.97 4.97 4.97	He	He	[He]	4.00
-1.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 -0.00 34.97 4.97 4.97 4.97 4.97	Ne	Ne	[Ne]	20.18
-1.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 -0.00 45.79 6.96 7.07 7.81 8.31		N2	N#N	28.01
1.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 -45.07 106.76 52.54 77.08 110.96 126.50		DTBS(1)	CC(C)(C)SC(C)(C)C	146.29
2.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 -4.90 49.18 8.18 8.88 10.93 12.29		H2S(2)	S	34.08
3.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 -3.80 69.99 21.54 31.20 46.91 54.64		C4H8(3)	C=C(C)C	56.11
4.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 -25.99 83.68 30.57 42.84 59.68 68.12		C4H9SH(4)	CC(C)(C)S	90.19
5.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 -32.50 70.43 23.06 35.25 54.22 63.87		C4H10(5)	CC(C)C	58.12
6.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 24.00 111.20 37.64 41.69 43.57 43.30		S8(6)	S1SSSSSSS1	256.52
7.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 57.33 108.00 28.71 30.13 30.79 29.66		S6J(7)	[S]SSSS[S]	192.39

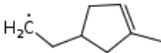
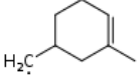
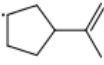
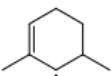
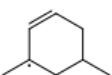
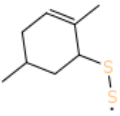
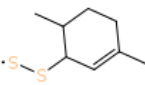
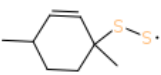
8.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 63.39 130.36 40.91 43.04 43.89 41.45		S8J(8)	[S]SSSSSS[S]	256.52
9.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 24.36 86.89 25.44 28.37 29.46 29.58		S6(9)	S1SSSSS1	192.39
10.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 51.27 85.64 16.51 17.22 17.69 17.87		S4J(10)	[S]SS[S]	128.26
11.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 34.84 71.81 16.82 18.89 19.53 19.72		S4(11)	S1SSS1	128.26
12.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 47.12 53.78 7.82 8.39 8.75 8.88		S2(12)	S=S	64.13
13.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 30.74 54.54 7.80 8.35 8.91 9.32		S2JJ(13)	[S][S]	64.13
14.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 23.01 89.28 29.76 40.99 55.88 63.48		C4H9S(14)	[CH2]C(C)(C)S	89.18
15.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 9.73 80.98 27.32 39.29 56.37 64.66		C4H9SJ(15)	CC(C)(C)[S]	89.18
16.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 33.30 46.76 7.74 7.50 7.90 8.33		HSJ(16)	[SH]	33.07
17.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 3.40 60.38 11.88 14.19 16.80 17.86		HSSH(17)	SS	66.15
20.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 11.90 74.29 22.20 31.86 49.45 58.50		C4H9(20)	CCC	57.11
22.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 34.89 46.37 9.34 10.62 13.45 15.09		CH3(22)	[CH3]	15.03
23.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 3.93 113.73 51.72 75.24 107.15 121.86		C8H17S(23)	[CH2]C(C)(C)SC(C)(C)C	145.29

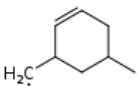
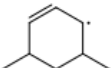
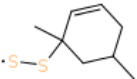
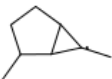
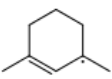
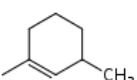
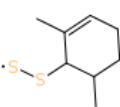
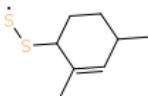
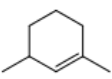
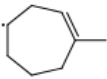
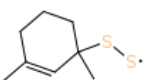
24.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 52.10 27.42 4.97 4.97 4.97 4.97		H(24)	[H]	1.01
25.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 25.23 60.88 9.61 10.78 12.21 12.98		HS2(25)	[S]S	65.14
33.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 32.30 69.61 20.96 30.41 44.29 51.20		C4H7(33)	[CH2]C(=C)C	55.10
35.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 45.06 100.81 29.37 39.53 56.41 64.55		C4H8S2(35)	CCCS[S]	120.24
44.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 -2.52 119.94 50.60 72.49 105.21 121.58		C8H17S(44)	CCCSC(C)(C)C	145.29
45.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 21.24 90.84 27.52 37.55 54.89 63.60		C4H9S(45)	CCCS	89.18
80.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 24.23 96.05 34.15 46.63 62.51 70.14		C4H9S2(80)	[CH2]C(C)(C)SS	121.24
86.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 49.97 72.25 17.66 26.89 42.31 50.05		C4H7(86)	C[C]1CC1	55.10
90.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 29.24 92.53 31.84 41.53 54.43 60.92		C4H7S2(90)	C=C(C)CS[S]	119.23
104.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 19.61 110.60 41.76 61.07 91.51 106.54		C8H15(104)	C=C(C)CCCC	111.20
124.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 3.28 104.50 40.92 60.27 89.36 102.83		C8H14(124)	C=C(C)CCC(=C)C	110.20
150.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 36.74 103.31 40.12 58.88 86.45 99.05		C8H13(150)	[CH2]C(C)=CCC(=C)C	109.19
154.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 44.95 97.22 35.98 56.22 91.61 106.40		C8H14(154)	C[C]1CCCCC1	110.20

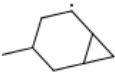
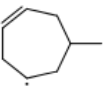
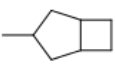
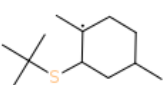
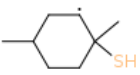
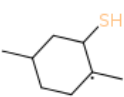
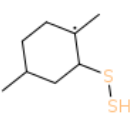
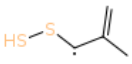
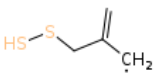
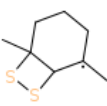
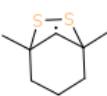
164.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(164)	[CH2]C(C)(CCC(=C)C)SC(C)(C)C	199.38
	10.84	147.86	71.32	104.43	149.22	169.99				
165.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(165)	C=C(C)CCCCSC(C)(C)C	199.38
	4.79	155.45	70.26	101.64	147.33	169.73				
166.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(166)	[CH2]C(C)(S)CCC(=C)C	143.27
	29.87	121.47	48.86	69.90	99.15	113.18				
167.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(167)	C=C(C)CCCCS	143.27
	28.55	126.34	47.27	66.65	97.02	111.80				
203.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(203)	CCCSS	121.24
	26.12	102.51	32.30	43.33	61.17	69.57				
441.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		C8H13(441)	C[C]1CC=C(C)CC1	109.19
	27.75	95.13	34.89	54.60	85.77	100.12				
443.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		C8H14(443)	CC1=CCC(C)CC1	110.20
	-16.65	89.89	35.74	58.07	90.41	105.62				
506.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		C8H13(506)	[CH2]C(C)=CC=C(C)C	109.19
	21.34	99.52	39.95	58.96	86.76	100.38				
514.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		C8H12(514)	[CH2]C(C)=CC=C([CH2])C	108.18
	49.23	97.40	38.10	57.06	84.07	97.95				
520.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		C8H13(520)	[CH2]C1(C)CC1C(=C)C	109.19
	56.62	98.07	37.90	58.77	86.46	99.28				
521.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		C8H12(521)	C=C(C)C=CC(=C)C	108.18
	23.44	93.86	40.26	58.96	83.03	94.93				
525.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(525)	C=C(C)CC=C(C)CS[S]	173.32
	33.68	126.22	50.88	70.21	96.21	108.90				
530.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(530)	C=C(C)CC(S[S])C(=C)C	173.32
	33.80	123.45	51.52	72.05	97.29	109.60				

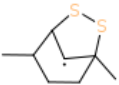
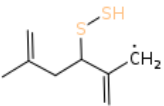
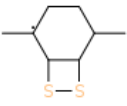
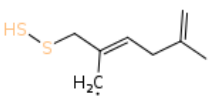
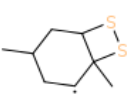
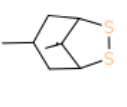
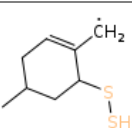
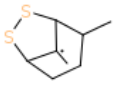
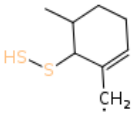
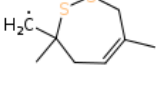
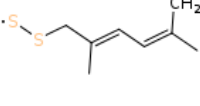
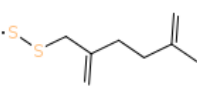
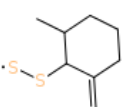


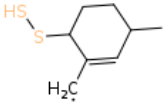
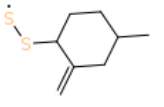
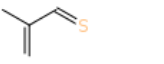
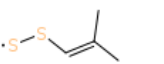
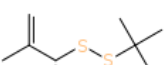
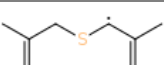
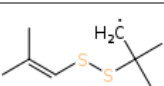
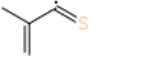
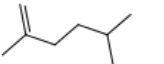
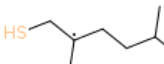
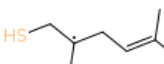
539.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 0.64 105.06 40.61 59.76 88.91 102.51		C8H14(539)	<chem>C=C(C)CC=C(C)C</chem>	110.20
649.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 40.16 91.96 32.86 54.87 87.43 101.19		C8H13(649)	<chem>C[C]1CCC2(C)CC12</chem>	109.19
735.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 8.10 86.02 34.88 54.51 82.61 95.80		C8H12(735)	<chem>CC1=CC=C(C)CC1</chem>	108.18
739.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 29.70 94.33 34.20 55.11 86.20 100.37		C8H13(739)	<chem>CC1=CCC(C)[CH]C1</chem>	109.19
740.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 16.25 86.08 34.21 55.98 87.24 101.78		C8H13(740)	<chem>CC1=C[CH]C(C)CC1</chem>	109.19
741.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 32.35 93.60 35.15 56.22 86.61 101.81		C8H13(741)	<chem>[CH2]C1CC=C(C)CC1</chem>	109.19
742.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 16.25 86.08 34.21 55.98 87.24 101.78		C8H13(742)	<chem>CC1[CH]CC(C)CC=1</chem>	109.19
744.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 19.45 88.13 35.16 57.27 87.84 102.18		C8H13(744)	<chem>[CH2]C1=CCC(C)CC1</chem>	109.19
807.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 35.29 94.11 36.30 57.39 86.62 99.74		C8H13(807)	<chem>[CH2]C1(C)C=C(C)CC1</chem>	109.19
817.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 37.26 91.23 32.37 55.35 87.92 101.64		C8H13(817)	<chem>CC1C[CH]C2(C)CC12</chem>	109.19
853.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 45.68 86.42 32.45 56.83 88.92 101.92		C8H13(853)	<chem>CC12[CH]C(C)(CC1)C2</chem>	109.19
978.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 16.93 104.81 46.45 71.16 100.38 112.17		S(978)	<chem>C=C1CCC(C)CC1S[S]</chem>	173.32

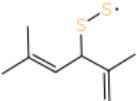
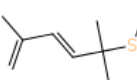
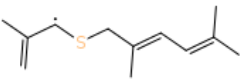
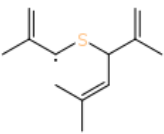
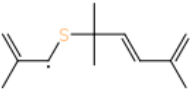
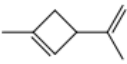
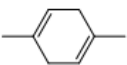
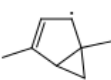
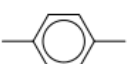
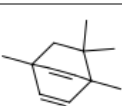
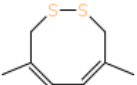
1217.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 8.78 34.94 40.84 60.25 89.52 102.55		S(1217)	C[C]1CCC2CC1C2	109.19
1218.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 27.74 86.07 36.48 58.63 89.04 101.93		S(1218)	CC12[CH]CC(CC1)C2	109.19
1311.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 37.15 97.92 35.57 56.21 85.80 99.66		S(1311)	[CH2]CC1CC=C(C)C1	109.19
1368.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 24.92 88.41 36.36 56.87 87.62 101.67		S(1368)	C[C]1CC2CCC1C2	109.19
1476.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 32.35 93.60 35.15 56.22 86.61 101.81		S(1476)	[CH2]C1CCC=C(C)C1	109.19
1487.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 35.80 101.33 33.22 53.51 84.59 100.05		S(1487)	C=C(C)C1C[CH]CC1	109.19
1507.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 -19.48 83.17 37.22 60.33 92.29 107.16		S(1507)	CC1CC2CCC1C2	110.20
1549.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 16.25 86.08 34.21 55.98 87.24 101.78		S(1549)	CC1[CH]C(C)CCC=1	109.19
1551.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 16.18 85.38 33.02 55.14 86.88 102.29		S(1551)	C[C]1C=CCC(C)C1	109.19
1769.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 39.29 93.50 32.07 53.63 86.46 101.17		S(1769)	C[C]1C2CC(C)CC12	109.19
1779.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 13.87 107.47 46.43 69.73 98.60 112.33		S(1779)	CC1=CCC(C)CC1S[S]	173.32
1837.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 13.87 107.47 46.43 69.73 98.60 112.33		S(1837)	CC1=CC(S[S])C(C)CC1	173.32
1840.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 15.02 108.30 43.34 67.04 98.53 112.00		S(1840)	CC1C=CC(C)(CC1)S[S]	173.32

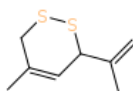
1965.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(1965)	<chem>[CH2]C1C=CCC(C)C1</chem>	109.19
	33.88	92.78	34.26	55.99	86.59	102.02				
1968.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(1968)	<chem>CC1[CH]C=CC(C)C1</chem>	109.19
	17.78	85.26	33.32	55.75	87.22	102.00				
1983.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(1983)	<chem>CC1CC=CC(C)(C1)S[S]</chem>	173.32
	14.77	108.30	43.34	67.00	98.56	111.99				
2061.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(2061)	<chem>C[C]1C2CCC(C)C12</chem>	109.19
	39.29	93.50	32.07	53.63	86.46	101.17				
2082.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(2082)	<chem>C[C]1C=C(C)CCC1</chem>	109.19
	14.90	86.20	33.91	55.41	86.88	102.08				
2083.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(2083)	<chem>[CH2]C1C=C(C)CCC1</chem>	109.19
	32.60	93.60	35.15	56.26	86.59	101.81				
2086.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(2086)	<chem>CC1=CCCC(C)C1S[S]</chem>	173.32
	13.87	107.47	46.43	69.73	98.60	112.33				
2089.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(2089)	<chem>CC1=CC(C)CCC1S[S]</chem>	173.32
	14.12	107.47	46.43	69.77	98.57	112.34				
2099.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(2099)	<chem>CC1=CC(C)CCC1</chem>	110.20
	-16.40	89.89	35.74	58.11	90.38	105.63				
2163.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(2163)	<chem>C[C]1CCCC2CC12</chem>	109.19
	37.73	92.63	31.30	52.94	86.91	101.73				
2260.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(2260)	<chem>CC1=CC[CH]CCC1</chem>	109.19
	36.17	91.86	31.96	57.45	84.45	100.61				
2306.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(2306)	<chem>CC12[CH]CC1CCC2</chem>	109.19
	8.55	32.67	41.14	61.95	91.01	102.96				
2392.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(2392)	<chem>CC1=CC(C)(CCC1)S[S]</chem>	173.32
	13.49	109.12	44.24	67.26	98.61	111.77				

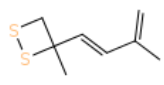
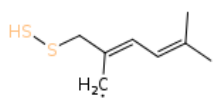
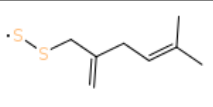
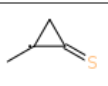
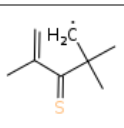
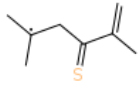
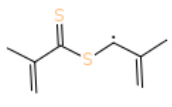
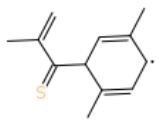
2490.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 33.73 91.90 30.81 53.42 87.40 102.18		S(2490)	CC1C[CH]C2CC2C1	109.19
2592.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 37.45 91.04 31.08 57.18 84.46 100.81		S(2592)	CC1C[CH]CC=CC1	109.19
2637.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 9.18 34.21 40.35 60.70 90.04 102.93		S(2637)	CC1CC2[CH]CC2C1	109.19
2919.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 -10.06 130.27 65.61 101.96 153.49 174.74		S(2919)	CC1C[CH]C(C)(CC1)SC(C)(C)C	199.38
2920.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 -13.07 131.93 65.90 101.02 153.34 174.90		S(2920)	C[C]1CCC(C)CC1SC(C)(C)C	199.38
2927.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 8.97 103.87 43.12 67.41 103.46 117.89		S(2927)	CC1C[CH]C(C)(S)CC1	143.27
2928.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 8.56 105.73 42.46 65.76 102.38 117.27		S(2928)	C[C]1CCC(C)CC1S	143.27
3191.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 12.47 116.39 47.64 72.16 108.84 123.25		S(3191)	C[C]1CCC(C)CC1SS	175.33
3383.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 40.11 94.89 31.59 42.85 56.33 62.40		S(3383)	C=C(C)[CH]SS	119.23
3384.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 46.39 92.47 34.19 44.54 56.64 62.49		S(3384)	[CH2]C(=C)CSS	119.23
4420.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 18.82 56.77 53.80 74.97 102.17 114.35		S(4420)	C[C]1CCCC2(C)SSC12	173.32
4421.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 19.23 54.91 54.48 76.57 103.43 114.87		S(4421)	CC12[CH]C(C)(CCC1)SS2	173.32

4688.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 20.77 55.97 53.13 75.36 102.88 114.45		S(4688)	CC1CCC2(C)[CH]C1SS2	173.32
4766.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 50.95 123.40 53.89 75.01 99.54 111.15		S(4766)	[CH2]C(=C)C(CC(=C)C)SS	173.32
4842.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 20.36 57.83 52.42 73.80 101.55 113.95		S(4842)	C[C]1CCC(C)C2SSC12	173.32
4998.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 50.83 126.17 53.23 73.20 98.43 110.46		S(4998)	[CH2]C(=CCC(=C)C)CSS	173.32
5073.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 20.77 55.97 53.13 75.36 102.88 114.45		S(5073)	CC1C[CH]C2(C)SSC2C1	173.32
5074.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 20.36 57.83 52.42 73.80 101.55 113.95		S(5074)	C[C]1C2CC(C)CC1SS2	173.32
5085.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 31.02 107.41 48.78 72.72 100.81 113.90		S(5085)	[CH2]C1=CCC(C)CC1SS	173.32
5345.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 20.36 57.83 52.42 73.80 101.55 113.95		S(5345)	C[C]1C2CCC(C)C1SS2	173.32
5358.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 31.02 107.41 48.78 72.72 100.81 113.90		S(5358)	[CH2]C1=CCCC(C)C1SS	173.32
5416.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 47.39 106.60 48.41 75.43 98.79 112.81		S(5416)	[CH2]C1(C)CC=C(C)CSS1	173.32
5433.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 54.37 120.69 50.20 69.41 94.12 106.74		S(5433)	[CH2]C(C)=CC=C(C)CS[S]	172.31
5528.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 36.32 127.04 51.14 70.75 96.61 109.21		S(5528)	C=C(C)CCC(=C)CS[S]	173.32
5657.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 16.93 104.81 46.45 71.16 100.38 112.17		S(5657)	C=C1CCCC(C)C1S[S]	173.32

5660.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(5660)	[CH2]C1=CC(C)CCC1SS	173.32
	31.27	107.41	48.78	72.76	100.79	113.91				
6088.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(6088)	C=C1CC(C)CCC1S[S]	173.32
	16.93	104.81	46.45	71.16	100.38	112.17				
6398.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(6398)	C=C(C)C=S	86.16
	28.99	76.76	22.49	32.72	46.31	51.98				
6410.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(6410)	CC(C)=CS[S]	119.23
	27.35	93.78	28.92	39.22	53.63	60.56				
6417.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(6417)	C=C(C)[CH]SSC(C)(C)C	175.33
	14.04	123.82	55.19	77.94	106.65	120.11				
6452.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(6452)	C=C(C)[CH]SCC(=C)C	141.25
	43.89	114.15	49.53	68.24	92.44	104.62				
7161.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(7161)	[CH2]C(C)(C)SSC=C(C)C	175.33
	31.33	130.02	54.70	76.21	104.99	118.65				
7670.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(7670)	C=C(C)[C]=S	85.15
	54.76	77.24	21.29	30.48	42.53	47.30				
8546.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(8546)	C=C(C)CCC(C)C	112.21
	-24.79	106.74	42.81	64.23	96.71	111.87				
8698.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(8698)	C[C](CS)CCC(C)C	145.29
	0.48	127.21	49.05	70.77	104.26	120.89				
8828.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(8828)	C[C](CS)CC=C(C)C	143.27
	25.21	125.51	46.94	66.14	96.68	111.49				
9017.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(9017)	CCC1CC1(C)CS	143.27
	34.71	114.33	44.59	66.29	98.67	112.93				
9203.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(9203)	CC(C)=CC=C(C)CS[S]	173.32
	26.48	121.43	52.02	71.38	96.66	109.23				

9208.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 33.34 102.40 48.41 68.09 94.21 105.74		S(9208)	<chem>C=C(C)C(C=C(C)C)S[S]</chem>	173.32
9210.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 28.32 119.58 49.22 70.50 97.78 109.63		S(9210)	<chem>C=C(C)C=CC(C)(C)S[S]</chem>	173.32
9515.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 41.13 143.06 69.71 98.06 134.69 152.90		S(9515)	<chem>C=C(C)[CH]SCC(C)=CC=C(C)C</chem>	195.34
9534.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 47.99 124.03 66.10 94.73 132.31 149.37		S(9534)	<chem>C=C(C)[CH]SC(C=C(C)C)C(=C)C</chem>	195.34
9554.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 42.97 141.21 66.93 97.12 135.89 153.27		S(9554)	<chem>C=C(C)[CH]SC(C)(C)C=CC(=C)C</chem>	195.34
9808.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 39.11 93.27 37.06 55.46 82.41 94.90		S(9808)	<chem>C=C(C)C1C=C(C)C1</chem>	108.18
10047.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 33.30 88.73 32.68 52.54 80.06 93.51		S(10047)	<chem>CC1[CH]C=C(C)CC=1</chem>	107.17
10429.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 18.06 20.34 38.18 58.49 84.44 95.25		S(10429)	<chem>CC1=C[CH]C2(C)CC12</chem>	107.17
10431.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 3.82 85.82 30.59 47.82 73.99 85.93		S(10431)	<chem>Cc1ccc(C)cc1</chem>	106.17
11190.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 -9.57 51.71 61.26 90.08 129.73 146.87		S(11190)	<chem>CC1=CC2C(C)=CC1CC2(C)C</chem>	162.27
11191.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 -7.51 49.67 59.09 90.96 131.75 147.45		S(11191)	<chem>CC12C=CC(C)(C=C1)C(C)(C)C2</chem>	162.27
11384.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 28.18 97.79 48.17 68.90 96.00 108.87		S(11384)	<chem>CC1=CC=C(C)CSSC1</chem>	172.31
11398.	H298 S298 Cp300 Cp500 Cp1000 Cp1500 24.62 81.63 47.60 68.82 96.78 106.86		S(11398)	<chem>C=C(C)C1C=C(C)CSS1</chem>	172.31



11414.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(11414)	<chem>C=C(C)C=CC1(C)CSS1</chem>	172.31
	43.10	108.29	46.80	68.37	95.60	107.07				
11955.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(11955)	<chem>[CH2]C(=CC=C(C)C)CSS</chem>	173.32
	35.43	122.39	53.13	73.22	98.87	111.77				
12040.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(12040)	<chem>C=C(CC=C(C)C)CS[S]</chem>	173.32
	33.68	126.22	50.88	70.21	96.21	108.90				
12964.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(12964)	<chem>C[C]1CC1=S</chem>	85.15
	52.73	41.96	14.60	24.52	37.46	44.35				
12992.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(12992)	<chem>[CH2]C(C)(C)C(=S)C(=C)C</chem>	141.25
	35.36	82.33	41.70	61.18	87.98	99.81				
12993.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(12993)	<chem>C=C(C)C(=S)CCC</chem>	141.25
	32.62	86.58	40.74	58.69	85.75	99.06				
13752.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(13752)	<chem>C=C(C)[CH]SC(=S)C(=C)C</chem>	171.30
	53.30	90.89	44.49	63.33	87.06	97.46				
14191.	H298	S298	Cp300	Cp500	Cp1000	Cp1500		S(14191)	<chem>C=C(C)C(=S)C1C=C(C)[CH]C=C1C</chem>	191.31
	53.28	95.25	52.12	79.09	116.41	134.07				