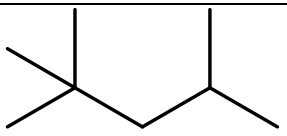
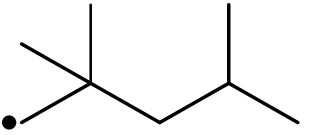
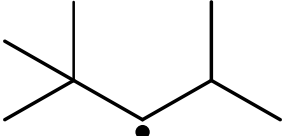
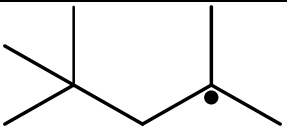
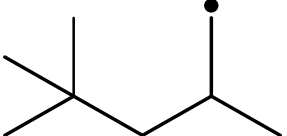
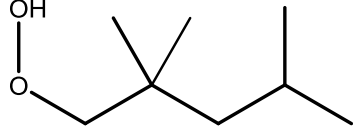
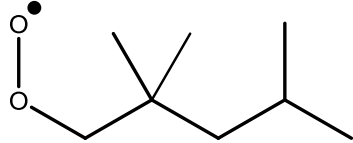
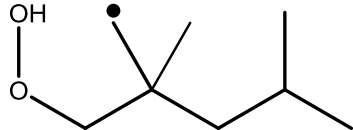
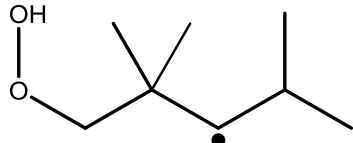


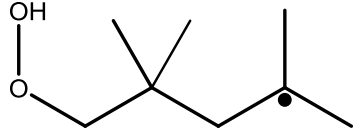
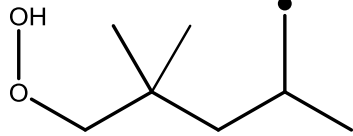
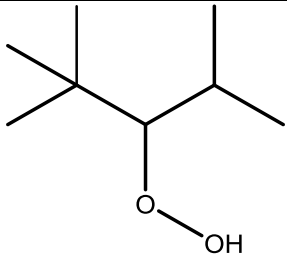
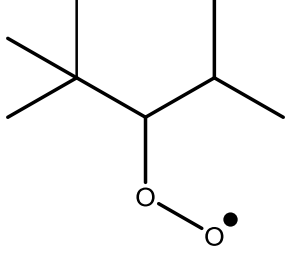
# Table S1

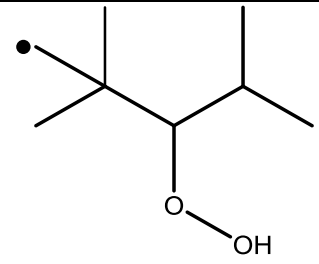
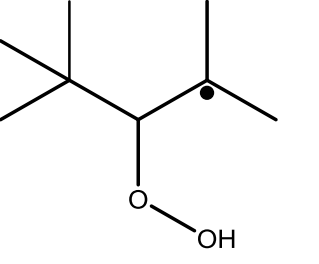
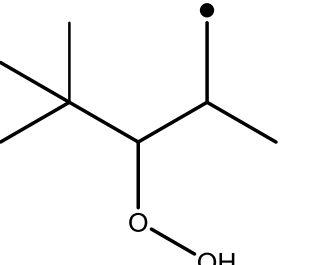
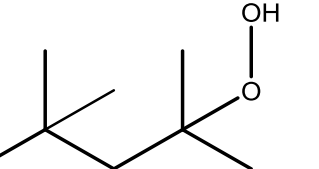
---

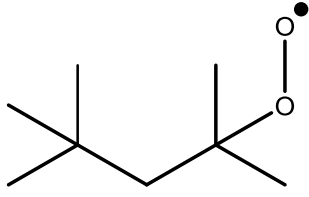
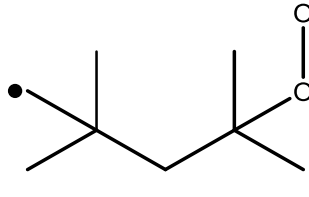
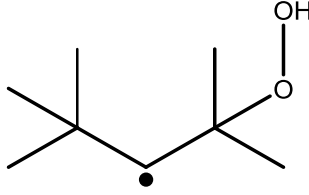
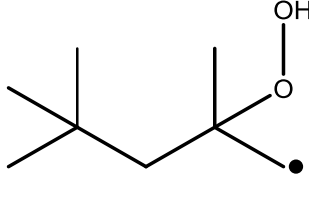
Species dictionary and THERM input

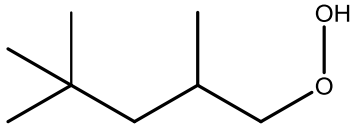
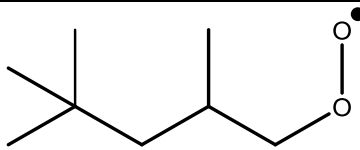
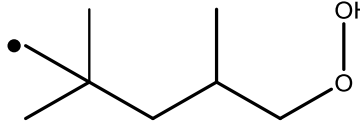
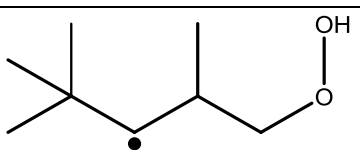
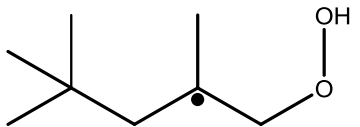
			Gauche	H15	Rotors	OI	Symm.	THERM groups
<b>Fuel and its radical</b>	IC8H18		3	1	7	0	729	UNITS:KCAL GROUPS 6 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   4 - C/C3/H - 1 2 - C/C4 - 1   5 - GAUCHE - 3 3 - C/C2/H2 - 1   6 - H15 - 1 Hf S Cp 300 400 500 600 800 1000 1500 -53.14 101.53 45.63 58.20 69.74 79.78 95.82 107.13 .00 CPINF = 144.06 NROTORS: 7 SYMMETRY 729
	AC8H17		2	1	7	0	162	UNITS:KCAL GROUPS 7 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   5 - GAUCHE - 2 2 - C/C4 - 1   6 - H15 - 1 3 - C/C2/H2 - 1   7 - P - 1 4 - C/C3/H - 1 Hf S Cp 300 400 500 600 800 1000 1500 -4.89 107.03 44.49 56.56 67.60 77.18 92.50 103.24 .00 CPINF = 138.10 NROTORS: 7 SYMMETRY 162
	BC8H17		3	1	7	0	729	UNITS:KCAL GROUPS 7 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   5 - GAUCHE - 3 2 - C/C4 - 1   6 - H15 - 1 3 - C/C2/H2 - 1   7 - S - 1 4 - C/C3/H - 1 Hf S Cp 300 400 500 600 800 1000 1500 -7.17 105.79 43.85 55.22 66.25 75.97 91.42 102.35 .00 CPINF = 138.10 NROTORS: 7 SYMMETRY 729
	CC8H17		3	1	7		1458	UNITS:KCAL GROUPS 6 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   4 - C/C3/H - 1 2 - C/C4 - 1   5 - GAUCHE - 3 3 - C/C2/H2 - 1   6 - T - 1 Hf S Cp 300 400 500 600 800 1000 1500 -10.22 105.71 44.05 55.08 65.83 75.48 91.22 102.35 .00 CPINF = 138.10 NROTORS: 7 SYMMETRY 1458
	DC8H17		2	1	7	0	486	UNITS:KCAL GROUPS 7 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   5 - GAUCHE - 2 2 - C/C4 - 1   6 - H15 - 1 3 - C/C2/H2 - 1   7 - P - 1

			Gauche	H15	Rotors	OI	Symm.	THERM groups
								4 - C/C3/H - 1 Hf S Cp 300 400 500 600 800 1000 1500 -4.89 104.85 44.49 56.56 67.60 77.18 92.50 103.24 .00 CPINF = 138.10 NROTORS: 7 SYMMETRY 486
<b>ROOH, RO2 and QOOH</b>	AC8H17OOH		3	0	9	1	81	UNITS:KCAL GROUPS 8 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   5 - C/C/H2/OO - 1 2 - C/C4 - 1   6 - OO/C/H - 1 3 - C/C2/H2 - 1   7 - GAUCHE - 3 4 - C/C3/H - 1   8 - OI - 1 Hf S Cp 300 400 500 600 800 1000 1500 -73.25 122.24 52.78 66.35 78.58 89.14 105.66 117.24 .00 CPINF = 153.99 NROTORS: 9 SYMMETRY 81
	AC8H17O2		3	0	9	1	81	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - OO/C/H - 1 2 - C/C4 - 1   7 - GAUCHE - 3 3 - C/C2/H2 - 1   8 - OI - 1 4 - C/C3/H - 1   9 - ALPEROX - 1 5 - C/C/H2/OO - 1 Hf S Cp 300 400 500 600 800 1000 1500 -40.08 121.76 51.61 64.57 76.30 86.40 102.41 113.56 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 81
	AC8H16OOH-A		2	0	9	1	54	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - GAUCHE - 2 2 - C/C4 - 1   7 - OI - 1 3 - C/C2/H2 - 1   8 - OO/C/H - 1 4 - C/C3/H - 1   9 - P - 1 5 - C/C/H2/OO - 1 Hf S Cp 300 400 500 600 800 1000 1500 -25.00 125.55 51.64 64.71 76.44 86.54 102.34 113.35 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 54
	AC8H16OOH-B		3	0	9	1	81	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - OO/C/H - 1 2 - C/C4 - 1   7 - GAUCHE - 3 3 - C/C2/H2 - 1   8 - OI - 1 4 - C/C3/H - 1   9 - S - 1 5 - C/C/H2/OO - 1 Hf S Cp 300 400 500 600 800 1000 1500 -27.28 126.50 51.00 63.37 75.09 85.33 101.26 112.46 .00 CPINF = 148.03

			Gauche	H15	Rotors	OI	Symm.	THERM groups
								NROTORS: 9 SYMMETRY 81
AC8H16OOH-C		3	0	9	1	162	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - OO/C/H - 1 2 - C/C4 - 1   7 - GAUCHE - 3 3 - C/C2/H2 - 1   8 - OI - 1 4 - C/C3/H - 1   9 - T - 1 5 - C/C/H2/OO - 1 Hf S Cp 300 400 500 600 800 1000 1500 -28.83 126.41 51.20 63.23 74.67 84.84 101.06 112.46 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 162	
AC8H16OOH-D		2	0	9	2	54	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - GAUCHE - 2 2 - C/C4 - 1   7 - OI - 1 3 - C/C2/H2 - 1   8 - OO/C/H - 1 4 - C/C3/H - 1   9 - P - 1 5 - C/C/H2/OO - 1 Hf S Cp 300 400 500 600 800 1000 1500 -25.00 125.55 51.64 64.71 76.44 86.54 102.34 113.35 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 54	
BC8H17OOH		3	1	9	2	729	UNITS:KCAL GROUPS 8 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   5 - OO/C/H - 1 2 - C/C4 - 1   6 - OI - 2 3 - C/C2/H/OO - 1   7 - H15 - 1 4 - C/C3/H - 1   8 - GAUCHE - 3 Hf S Cp 300 400 500 600 800 1000 1500 -75.77 117.80 53.99 67.49 79.50 90.01 105.93 117.17 .00 CPINF = 153.99 NROTORS: 9 SYMMETRY 729	
BC8H17O2		3	1	9	2	729	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   6 - OI - 2 2 - C/C4 - 1   7 - H15 - 1 3 - C/C2/H/OO - 1   8 - GAUCHE - 3 4 - C/C3/H - 1   9 - ALPEROX - 1 5 - OO/C/H - 1 Hf S Cp 300 400 500 600 800 1000 1500 -42.60 117.32 52.82 65.71 77.22 87.27 102.68 113.49 .00 CPINF = 148.03 NROTORS: 9	

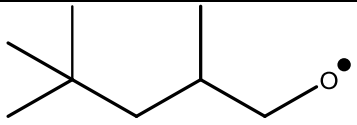
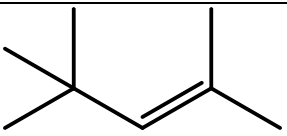
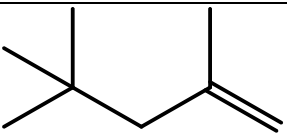
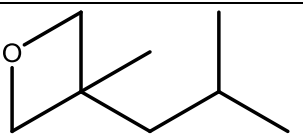
			Gauche	H15	Rotors	OI	Symm.	THERM groups
								SYMMETRY 729
BC8H16OOH-A		2	1	9	2	162	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   6 - OI - 2 2 - C/C4 - 1   7 - H15 - 1 3 - C/C2/H/OO - 1   8 - GAUCHE - 2 4 - C/C3/H - 1   9 - P - 1 5 - OO/C/H - 1 Hf S Cp 300 400 500 600 800 1000 1500 -27.52 123.30 52.85 65.85 77.36 87.41 102.61 113.28 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 162	
BC8H16OOH-C		3	0	9	2	1458	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   6 - OI - 2 2 - C/C4 - 1   7 - H15 - 1 3 - C/C2/H/OO - 1   8 - GAUCHE - 3 4 - C/C3/H - 1   9 - T - 1 5 - OO/C/H - 1 Hf S Cp 300 400 500 600 800 1000 1500 -31.35 121.98 52.41 64.37 75.59 85.71 101.33 112.39 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 1458	
BC8H16OOH-D		2	1	9	3	486	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   6 - OI - 3 2 - C/C4 - 1   7 - H15 - 1 3 - C/C2/H/OO - 1   8 - GAUCHE - 2 4 - C/C3/H - 1   9 - P - 1 5 - OO/C/H - 1 Hf S Cp 300 400 500 600 800 1000 1500 -27.52 122.49 52.85 65.85 77.36 87.41 102.61 113.28 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 486	
CC8H17OOH		3	1	9	1	729	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   6 - H15 - 1 2 - C/C4 - 1   7 - OI - 1 3 - GAUCHE - 3   8 - OO/C/H - 1 4 - C/C2/H2 - 1   9 - DUM1 - 2 5 - C/C3/OO - 1 Hf S Cp 300 400 500 600 800 1000 1500 -78.10 114.30 53.81 67.12 79.04 89.39 105.62 117.07 .00 CPINF = 153.99 NROTORS: 9 SYMMETRY 729	

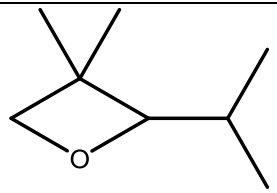
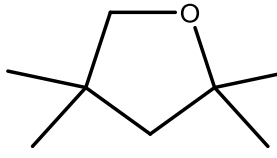
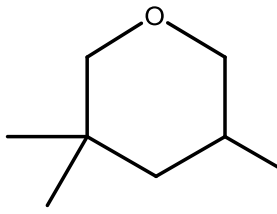
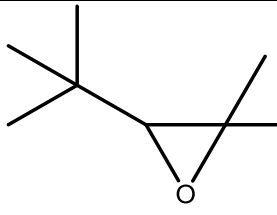
			Gauche	H15	Rotors	OI	Symm.	THERM groups
CC8H17O2		3	1	9	1	729	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   6 - H15 - 1 2 - C/C4 - 1   7 - OI - 1 3 - GAUCHE - 3   8 - OO/C/H - 1 4 - C/C2/H2 - 1   9 - ALPEROX - 1 5 - C/C3/OO - 1 Hf S Cp 300 400 500 600 800 1000 1500 -46.93 113.82 52.64 65.34 76.76 86.65 102.37 113.39 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 729	
CC8H16OOH-A		2	1	9	1	162	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   6 - H15 - 1 2 - C/C4 - 1   7 - OI - 1 3 - GAUCHE - 2   8 - OO/C/H - 1 4 - C/C2/H2 - 1   9 - DUM1 - 2 5 - C/C3/OO - 1   10 - P - 1 Hf S Cp 300 400 500 600 800 1000 1500 -29.85 119.80 52.67 65.48 76.90 86.79 102.30 113.18 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 162	
CC8H16OOH-B		3	1	9	1	729	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   6 - H15 - 1 2 - C/C4 - 1   7 - OI - 1 3 - GAUCHE - 3   8 - OO/C/H - 1 4 - C/C2/H2 - 1   9 - DUM1 - 2 5 - C/C3/OO - 1   10 - S - 1 Hf S Cp 300 400 500 600 800 1000 1500 -32.13 118.56 52.03 64.14 75.55 85.58 101.22 112.29 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 729	
CC8H16OOH-D		2	1	9	2	486	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   6 - H15 - 1 2 - C/C4 - 1   7 - OI - 2 3 - GAUCHE - 2   8 - OO/C/H - 1 4 - C/C2/H2 - 1   9 - DUM1 - 2 5 - C/C3/OO - 1   10 - P - 1 Hf S Cp 300 400 500 600 800 1000 1500 -29.85 118.99 52.67 65.48 76.90 86.79 102.30 113.18 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 486	

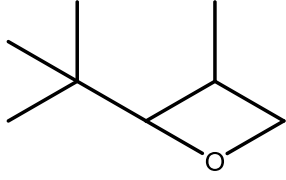
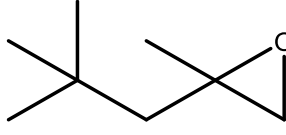
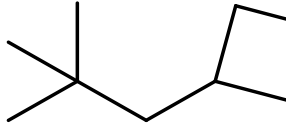
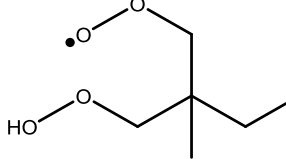
			Gauche	H15	Rotors	OI	Symm.	THERM groups
DC8H17OOH		3	0	9	2	243	UNITS:KCAL GROUPS 8 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   5 - C/C/H2/OO - 1 2 - C/C4 - 1   6 - OO/C/H - 1 3 - C/C2/H2 - 1   7 - OI - 2 4 - C/C3/H - 1   8 - GAUCHE - 3 Hf S Cp 300 400 500 600 800 1000 1500 -73.25 121.43 52.78 66.35 78.58 89.14 105.66 117.24 .00 CPINF = 153.99 NROTORS: 9 SYMMETRY 243	
DC8H17O2		3	0	9	2	243	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - OO/C/H - 1 2 - C/C4 - 1   7 - OI - 2 3 - C/C2/H2 - 1   8 - GAUCHE - 3 4 - C/C3/H - 1   9 - ALPEROX - 1 5 - C/C/H2/OO - 1 Hf S Cp 300 400 500 600 800 1000 1500 -40.08 120.95 51.61 64.57 76.30 86.40 102.41 113.56 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 243	
DC8H16OOH-A		2	0	9	2	54	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - OO/C/H - 1 2 - C/C4 - 1   7 - OI - 2 3 - C/C2/H2 - 1   8 - GAUCHE - 2 4 - C/C3/H - 1   9 - P - 1 5 - C/C/H2/OO - 1 Hf S Cp 300 400 500 600 800 1000 1500 -25.00 126.92 51.64 64.71 76.44 86.54 102.34 113.35 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 54	
DC8H16OOH-B		3	0	9	2	243	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - OO/C/H - 1 2 - C/C4 - 1   7 - OI - 2 3 - C/C2/H2 - 1   8 - GAUCHE - 3 4 - C/C3/H - 1   9 - S - 1 5 - C/C/H2/OO - 1 Hf S Cp 300 400 500 600 800 1000 1500 -27.28 125.69 51.00 63.37 75.09 85.33 101.26 112.46 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 243	
DC8H16OOH-C		3	0	9	1	243	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - OO/C/H - 1	

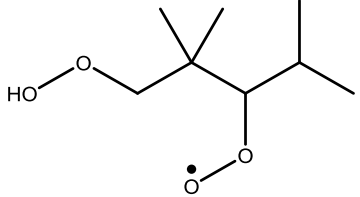
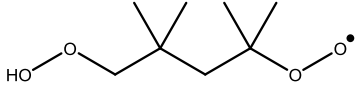
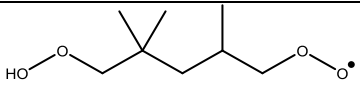
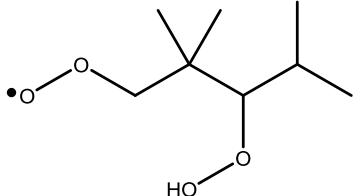
			Gauche	H15	Rotors	OI	Symm.	THERM groups
								2 - C/C4 - 1   7 - OI - 1 3 - C/C2/H2 - 1   8 - GAUCHE - 3 4 - C/C3/H - 1   9 - T - 1 5 - C/C/H2/OO - 1 Hf S Cp 300 400 500 600 800 1000 1500 -28.83 125.61 51.20 63.23 74.67 84.84 101.06 112.46 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 243
	DC8H16OOH-D		2	0	9	2	162	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - OO/C/H - 1 2 - C/C4 - 1   7 - OI - 2 3 - C/C2/H2 - 1   8 - GAUCHE - 2 4 - C/C3/H - 1   9 - P - 1 5 - C/C/H2/OO - 1 Hf S Cp 300 400 500 600 800 1000 1500 -25.00 124.74 51.64 64.71 76.44 86.54 102.34 113.35 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 162
Alkoxies	AC8H17O		3	1	8	0	81	UNITS:KCAL GROUPS 8 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H2/O - 1   5 - C/C2/H2 - 1 2 - O/C/H - 1   6 - C/C3/H - 1 3 - C/C4 - 1   7 - GAUCHE - 3 4 - C/C/H3 - 3   8 - ALKOXY - 1 Hf S Cp 300 400 500 600 800 1000 1500 -27.92 82.85 42.76 53.32 63.34 71.86 85.38 94.54 .00 CPINF = 143.06 NROTORS: 8 SYMMETRY 81
	BC8H17O		3	1	8	1	729	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   6 - OI - 1 2 - C/C4 - 1   7 - H15 - 1 3 - C/C2/H/O - 1   8 - GAUCHE - 3 4 - O/C/H - 1   9 - ALKOXY - 1 5 - C/C3/H - 1 Hf S Cp 300 400 500 600 800 1000 1500 -40.46 109.06 49.67 61.81 73.22 82.97 98.36 108.95 .00 CPINF = 143.06 NROTORS: 8 SYMMETRY 729
	CC8H17O		3	1	8	0	729	UNITS:KCAL GROUPS 8 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   5 - O/C/H - 1 2 - C/C4 - 1   6 - H15 - 1 3 - C/C2/H2 - 1   7 - GAUCHE - 3 4 - C/C3/O - 1   8 - ALKOXY - 1 Hf S Cp 300 400 500 600 800 1000 1500

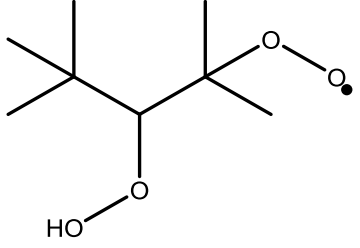
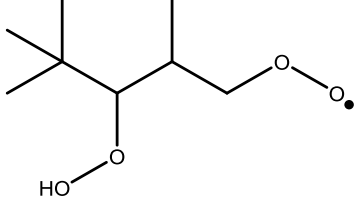
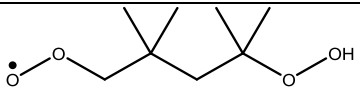
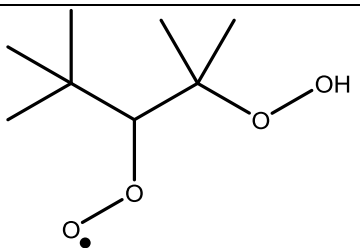


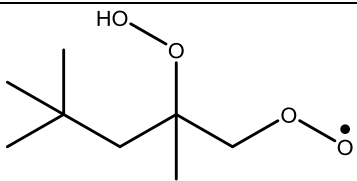
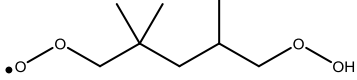
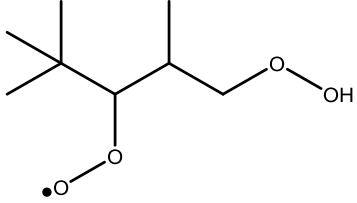
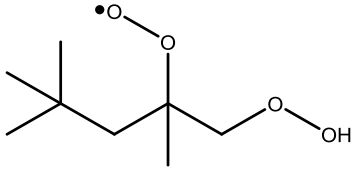
			Gauche	H15	Rotors	OI	Symm.	THERM groups
								-42.93 107.83 50.05 61.59 72.74 82.54 98.63 109.74 131.78 CPINF = 143.06 NROTORS: 8 SYMMETRY 729
	DC8H17O		3	0	8	1	243	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C3/H - 4   6 - O/C/H - 1 2 - C/C4 - 1   7 - GAUCHE - 3 3 - C/C2/H2 - 1   8 - OI - 1 4 - C/C3/H - 1   9 - ALKOXY - 1 5 - C/C/H2/O - 1 Hf S Cp 300 400 500 600 800 1000 1500 -6.25 -54.75 43.82 57.30 67.74 74.92 85.74 91.85 .00 CPINF = 143.06 NROTORS: 8 SYMMETRY 243
Olefins	IC8H16		1	1	6	0	729	UNITS:KCAL GROUPS 7 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/CD/H3 - 2   5 - C/C/H3 - 3 2 - CD/C2 - 1   6 - GAUCHE - 1 3 - CD/C/H - 1   7 - H15 - 1 4 - C/C3/CD - 1 Hf S Cp 300 400 500 600 800 1000 1500 -26.61 99.19 42.83 54.34 64.73 73.60 87.05 96.94 111.51 CPINF = 133.13 NROTORS: 6 SYMMETRY 729
	JC8H16		2	0	6	0	243	UNITS:KCAL GROUPS 7 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - CD/H2 - 1   5 - C/C4 - 1 2 - CD/C2 - 1   6 - C/C/H3 - 3 3 - C/CD/H3 - 1   7 - GAUCHE - 2 4 - C/C/CD/H2 - 1 Hf S Cp 300 400 500 600 800 1000 1500 -27.37 100.12 42.42 53.81 64.46 73.88 88.94 99.54 120.20 CPINF = 133.13 NROTORS: 6 SYMMETRY 243
Cyclic ethers	IC8ETERAA		3	0	5	0	27	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - O/C2 - 1 2 - C/C3/H - 1   7 - CY/C3O - 1 3 - C/C2/H2 - 1   8 - GAUCHE - 3 4 - C/C4 - 1   9 - DUM2 - 4 5 - C/C/H2/O - 2 Hf S Cp 300 400 500 600 800 1000 1500 -53.41 103.16 41.42 54.60 67.19 77.67 93.06 103.81 .00 CPINF = 140.08 NROTORS: 5 SYMMETRY 27

			Gauche	H15	Rotors	OI	Symm.	THERM groups
IC8ETERAB		3	0	5	1	81	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - C/C4 - 1 2 - C/C3/H - 1   7 - CY/C3O - 1 3 - C/C2/H/O - 1   8 - GAUCHE - 3 4 - O/C2 - 1   9 - OI - 1 5 - C/C/H2/O - 1   10 - DUM2 - 4 Hf S Cp 300 400 500 600 800 1000 1500 -57.44 101.27 42.11 55.35 67.83 78.16 93.20 103.63 .00 CPINF = 140.08 NROTORS: 5 SYMMETRY 81	
IC8ETERAC		2	0	4	0	81	UNITS:KCAL GROUPS 8 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   5 - C/C2/H2 - 1 2 - C/C4 - 1   6 - C/C3/O - 1 3 - C/C/H2/O - 1   7 - CY/C4O - 1 4 - O/C2 - 1   8 - GAUCHE - 2 Hf S Cp 300 400 500 600 800 1000 1500 -76.74 98.01 40.64 53.70 66.32 77.03 93.23 104.46 .00 CPINF = 141.08 NROTORS: 4 SYMMETRY 81	
IC8ETERAD		1	0	3	1	27	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - C/C/H2/O - 2 2 - C/C3/H - 1   7 - CY/C5O - 1 3 - C/C2/H2 - 1   8 - GAUCHE - 1 4 - C/C4 - 1   9 - OI - 1 5 - O/C2 - 1 Hf S Cp 300 400 500 600 800 1000 1500 -75.30 93.16 39.48 53.40 66.65 77.71 93.95 105.23 .00 CPINF = 142.07 NROTORS: 3 SYMMETRY 27	
IC8ETERBC		3	0	6	1	729	UNITS:KCAL GROUPS 8 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   5 - O/C2 - 1 2 - C/C4 - 1   6 - CY/C2O - 1 3 - C/C2/H/O - 1   7 - GAUCHE - 3 4 - C/C3/O - 1   8 - OI - 1 Hf S Cp 300 400 500 600 800 1000 1500 -58.20 98.49 45.18 57.50 69.23 79.13 94.01 104.34 .00 CPINF = 139.09 NROTORS: 6 SYMMETRY 729	

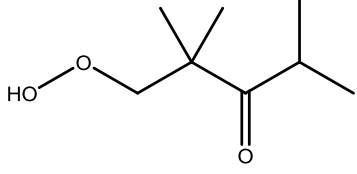
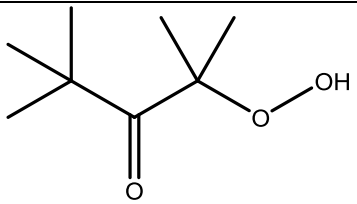
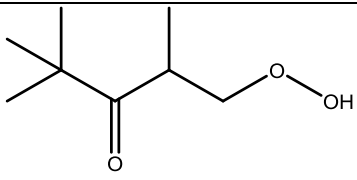
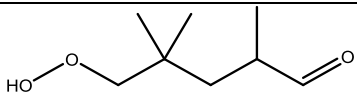
			Gauche	H15	Rotors	OI	Symm.	THERM groups
	IC8ETERBD		3	0	5	2	243	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - O/C2 - 1 2 - C/C4 - 1   7 - CY/C3O - 1 3 - C/C2/H/O - 1   8 - GAUCHE - 3 4 - C/C3/H - 1   9 - OI - 2 5 - C/C/H2/O - 1   10 - DUM2 - 4 Hf S Cp 300 400 500 600 800 1000 1500 -57.44 100.45 42.11 55.35 67.83 78.16 93.20 103.63 .00 CPINF = 140.08 NROTORS: 5 SYMMETRY 243
	IC8ETERCD		3	0	6	1	243	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - O/C2 - 1 2 - C/C4 - 1   7 - CY/C2O - 1 3 - C/C2/H2 - 1   8 - GAUCHE - 3 4 - C/C3/O - 1   9 - OI - 1 5 - C/C/H2/O - 1 Hf S Cp 300 400 500 600 800 1000 1500 -54.17 101.75 44.49 56.75 68.59 78.64 93.87 104.52 .00 CPINF = 139.09 NROTORS: 6 SYMMETRY 243
	IC8ETERDD		3	0	5	0	81	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - O/C2 - 1 2 - C/C4 - 1   7 - CY/C3O - 1 3 - C/C2/H2 - 1   8 - GAUCHE - 3 4 - C/C3/H - 1   9 - DUM2 - 4 5 - C/C/H2/O - 2 Hf S Cp 300 400 500 600 800 1000 1500 -53.41 100.98 41.42 54.60 67.19 77.67 93.06 103.81 .00 CPINF = 140.08 NROTORS: 5 SYMMETRY 81
OOQOOH	AC8H16OOH-AO2		3	0	11	3	27	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - OO/C/H - 2 2 - C/C3/H - 1   7 - OI - 3 3 - C/C2/H2 - 1   8 - GAUCHE - 3 4 - C/C4 - 1   9 - ALPEROX - 1 5 - C/C/H2/OO - 2 Hf S Cp 300 400 500 600 800 1000 1500 -58.69 141.65 58.76 72.72 85.14 95.76 112.25 123.67 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 27

			Gauche	H15	Rotors	OI	Symm.	THERM groups
	AC8H16OOH-BO2		3	0	11	3	81	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - C/C3/H - 1 2 - C/C4 - 1   7 - GAUCHE - 3 3 - C/C/H2/OO - 1   8 - OI - 3 4 - OO/C/H - 2   9 - ALPEROX - 1 5 - C/C2/H/OO - 1 Hf S Cp 300 400 500 600 800 1000 1500 -62.71 138.03 59.97 73.86 86.06 96.63 112.52 123.60 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 81
	AC8H16OOH-CO2		3	0	11	2	81	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - C/C3/OO - 1 2 - C/C4 - 1   7 - OI - 2 3 - C/C2/H2 - 1   8 - GAUCHE - 3 4 - C/C/H2/OO - 1   9 - ALPEROX - 1 5 - OO/C/H - 2 Hf S Cp 300 400 500 600 800 1000 1500 -67.04 134.53 59.79 73.49 85.60 96.01 112.21 123.50 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 81
	AC8H16OOH-DO2		3	0	11	3	27	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - OO/C/H - 2 2 - C/C4 - 1   7 - OI - 3 3 - C/C2/H2 - 1   8 - GAUCHE - 3 4 - C/C3/H - 1   9 - ALPEROX - 1 5 - C/C/H2/OO - 2 Hf S Cp 300 400 500 600 800 1000 1500 -58.69 141.65 58.76 72.72 85.14 95.76 112.25 123.67 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 27
	BC8H16OOH-AO2		3	0	11	3	81	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - C/C3/H - 1 2 - C/C4 - 1   7 - OI - 3 3 - C/C/H2/OO - 1   8 - GAUCHE - 3 4 - OO/C/H - 2   9 - ALPEROX - 1 5 - C/C2/H/OO - 1 Hf S Cp 300 400 500 600 800 1000 1500 -62.71 138.03 59.97 73.86 86.06 96.63 112.52 123.60 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 81

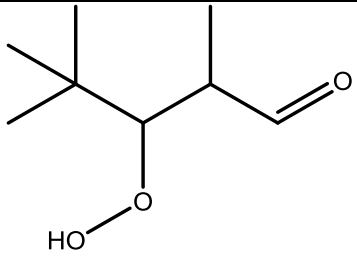
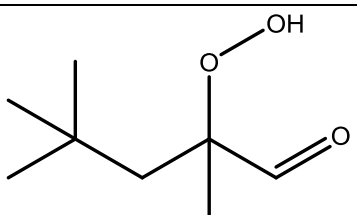
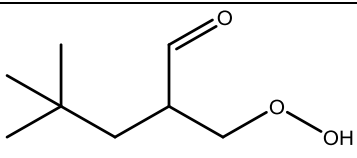
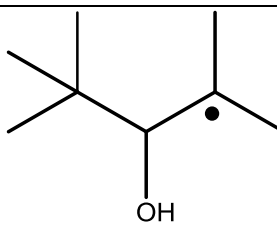
			Gauche	H15	Rotors	OI	Symm.	THERM groups
BC8H16OOH-CO2		3	1	11	3	729	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   6 - GAUCHE - 3 2 - C/C4 - 1   7 - OI - 3 3 - C/C2/H/OO - 1   8 - H15 - 1 4 - OO/C/H - 2   9 - ALPEROX - 1 5 - C/C3/OO - 1 Hf S Cp 300 400 500 600 800 1000 1500 -69.56 130.09 61.00 74.63 86.52 96.88 112.48 123.43 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 729	
BC8H16OOH-DO2		3	0	11	4	243	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - C/C/H2/OO - 1 2 - C/C4 - 1   7 - GAUCHE - 3 3 - C/C2/H/OO - 1   8 - OI - 4 4 - OO/C/H - 2   9 - ALPEROX - 1 5 - C/C3/H - 1 Hf S Cp 300 400 500 600 800 1000 1500 -62.71 137.22 59.97 73.86 86.06 96.63 112.52 123.60 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 243	
CC8H16OOH-AO2		3	0	11	2	81	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - C/C3/OO - 1 2 - C/C4 - 1   7 - OI - 2 3 - C/C2/H2 - 1   8 - GAUCHE - 3 4 - C/C/H2/OO - 1   9 - DUM1 - 2 5 - OO/C/H - 2   10 - ALPEROX - 1 Hf S Cp 300 400 500 600 800 1000 1500 -65.04 134.53 59.79 73.49 85.60 96.01 112.21 123.50 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 81	
CC8H16OOH-BO2		3	1	11	3	729	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   6 - GAUCHE - 3 2 - C/C4 - 1   7 - OI - 3 3 - C/C2/H/OO - 1   8 - H15 - 1 4 - OO/C/H - 2   9 - DUM1 - 2 5 - C/C3/OO - 1   10 - ALPEROX - 1 Hf S Cp 300 400 500 600 800 1000 1500 -67.56 130.09 61.00 74.63 86.52 96.88 112.48 123.43 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 729	

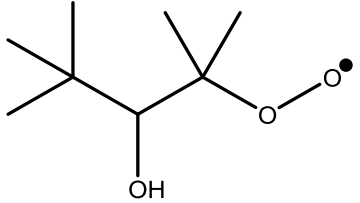
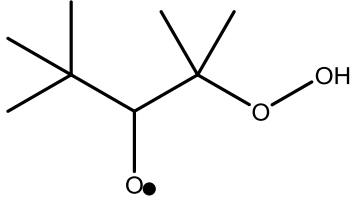
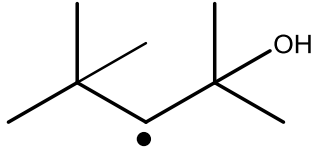
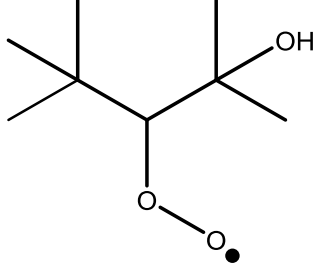
			Gauche	H15	Rotors	OI	Symm.	THERM groups
	CC8H16OOH-DO2		3	0	11	3	243	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - C/C/H2/OO - 1 2 - C/C4 - 1   7 - OI - 3 3 - C/C2/H2 - 1   8 - GAUCHE - 3 4 - C/C3/OO - 1   9 - DUM1 - 2 5 - OO/C/H - 2   10 - ALPEROX - 1 Hf S Cp 300 400 500 600 800 1000 1500 -65.04 133.72 59.79 73.49 85.60 96.01 112.21 123.50 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 243
	DC8H16OOH-AO2		3	0	11	3	27	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - OO/C/H - 2 2 - C/C4 - 1   7 - OI - 3 3 - C/C2/H2 - 1   8 - GAUCHE - 3 4 - C/C3/H - 1   9 - ALPEROX - 1 5 - C/C/H2/OO - 2 Hf S Cp 300 400 500 600 800 1000 1500 -58.69 141.65 58.76 72.72 85.14 95.76 112.25 123.67 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 27
	DC8H16OOH-BO2		3	0	11	4	243	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - C/C/H2/OO - 1 2 - C/C4 - 1   7 - OI - 4 3 - C/C2/H/OO - 1   8 - GAUCHE - 3 4 - OO/C/H - 2   9 - ALPEROX - 1 5 - C/C3/H - 1 Hf S Cp 300 400 500 600 800 1000 1500 -62.71 137.22 59.97 73.86 86.06 96.63 112.52 123.60 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 243
	DC8H16OOH-CO2		3	0	11	3	243	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - C/C/H2/OO - 1 2 - C/C4 - 1   7 - OI - 3 3 - C/C2/H2 - 1   8 - GAUCHE - 3 4 - C/C3/OO - 1   9 - ALPEROX - 1 5 - OO/C/H - 2 Hf S Cp 300 400 500 600 800 1000 1500 -67.04 133.72 59.79 73.49 85.60 96.01 112.21 123.50 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 243

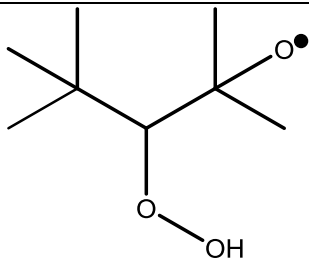
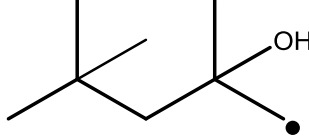
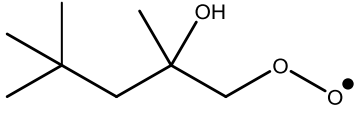
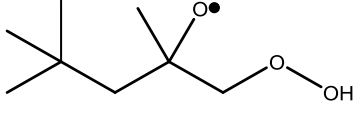
			Gauche	H15	Rotors	OI	Symm.	THERM groups
	DC8H16OOH-DO2		3	0	11	3	81	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - OO/C/H - 2 2 - C/C4 - 1   7 - OI - 3 3 - C/C2/H2 - 1   8 - GAUCHE - 3 4 - C/C3/H - 1   9 - ALPEROX - 1 5 - C/C/H2/OO - 2 Hf S Cp 300 400 500 600 800 1000 1500 -58.69 139.47 58.76 72.72 85.14 95.76 112.25 123.67 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 81
<b>KHP</b>	IC8KETAA		3	0	9	2	27	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - OO/C/H - 1 2 - C/C3/CO - 1   7 - CO/C/H - 1 3 - C/C2/H2 - 1   8 - OI - 2 4 - C/C3/H - 1   9 - GAUCHE - 3 5 - C/C/H2/OO - 1 Hf S Cp 300 400 500 600 800 1000 1500 -94.16 131.61 53.08 65.83 77.02 86.50 100.47 110.90 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 27
	IC8KETAB		3	0	9	2	81	UNITS:KCAL GROUPS 8 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   5 - OO/C/H - 1 2 - C/C3/CO - 1   6 - C/C3/H - 1 3 - CO/C/H - 1   7 - OI - 2 4 - C/C2/H/OO - 1   8 - GAUCHE - 3 Hf S Cp 300 400 500 600 800 1000 1500 -98.18 127.99 54.29 66.97 77.94 87.37 100.74 110.83 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 81
	IC8KETAC		3	0	9	1	81	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - C/C2/H2 - 1 2 - GAUCHE - 3   7 - C/C3/OO - 1 3 - OI - 1   8 - OO/C/H - 1 4 - C/C3/CO - 1   9 - DUM1 - 2 5 - CO/C/H - 1 Hf S Cp 300 400 500 600 800 1000 1500 -100.51 124.49 54.11 66.60 77.48 86.75 100.43 110.73 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 81
	IC8KETAD		3	0	9	2	27	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - C/C/H2/OO - 1

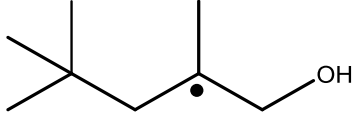
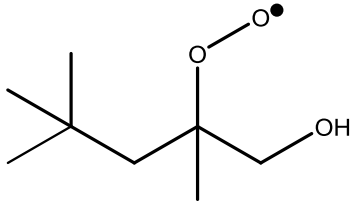
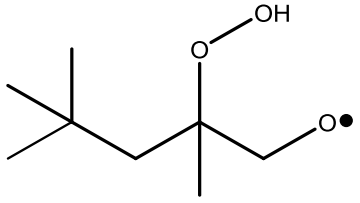
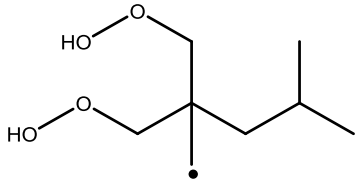
			Gauche	H15	Rotors	OI	Symm.	THERM groups
								2 - C/C3/CO - 1   7 - OO/C/H - 1 3 - CO/C/H - 1   8 - OI - 2 4 - C/C2/H2 - 1   9 - GAUCHE - 3 5 - C/C3/H - 1 Hf S Cp 300 400 500 600 800 1000 1500 -94.16 131.61 53.08 65.83 77.02 86.50 100.47 110.90 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 27
IC8KETBA		3	0	9	1	81	UNITS:KCAL GROUPS 8 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   5 - CO/C2 - 1 2 - C/C3/CO - 1   6 - C/C2/CO/H - 1 3 - C/C/H2/OO - 1   7 - OI - 1 4 - OO/C/H - 1   8 - GAUCHE - 3 Hf S Cp 300 400 500 600 800 1000 1500 -101.97 129.33 52.64 64.25 74.99 84.29 98.18 108.58 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 81	
IC8KETBC		3	1	9	1	729	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   6 - O/H/O - 1 2 - C/C3/CO - 1   7 - OI - 1 3 - CO/C2 - 1   8 - GAUCHE - 3 4 - C/C2/CO/O - 1   9 - H15 - 1 5 - O/C/O - 1   10 - DUM1 - 2 Hf S Cp 300 400 500 600 800 1000 1500 -102.53 123.18 53.60 65.99 77.20 86.84 101.00 111.51 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 729	
IC8KETBD		3	0	9	2	243	UNITS:KCAL GROUPS 8 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   5 - C/C/H2/OO - 1 2 - C/C3/CO - 1   6 - OO/C/H - 1 3 - CO/C2 - 1   7 - OI - 2 4 - C/C2/CO/H - 1   8 - GAUCHE - 3 Hf S Cp 300 400 500 600 800 1000 1500 -101.97 128.51 52.64 64.25 74.99 84.29 98.18 108.58 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 243	
IC8KETDA		3	0	9	2	27	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - C/C2/CO/H - 1 2 - C/C4 - 1   7 - CO/C/H - 1 3 - C/C/H2/OO - 1   8 - OI - 2 4 - OO/C/H - 1   9 - GAUCHE - 3 5 - C/C2/H2 - 1 Hf S Cp 300 400 500 600 800 1000 1500	



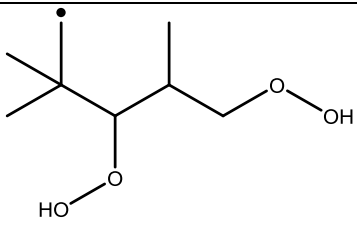
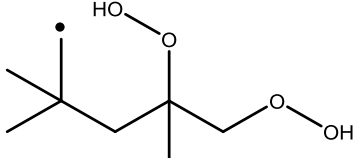
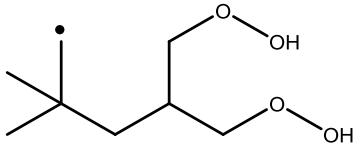
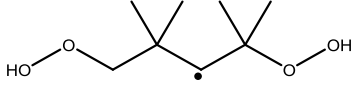
			Gauche	H15	Rotors	OI	Symm.	THERM groups
								-93.22 129.89 53.34 65.70 77.23 87.54 103.28 114.34 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 27
	IC8KETDB		3	0	9	3	243	UNITS:KCAL GROUPS 8 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   5 - C/C2/CO/H - 1 2 - C/C4 - 1   6 - CO/C/H - 1 3 - C/C2/H/OO - 1   7 - OI - 3 4 - OO/C/H - 1   8 - GAUCHE - 3 Hf S Cp 300 400 500 600 800 1000 1500 -97.24 125.45 54.55 66.84 78.15 88.41 103.55 114.27 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 243
	IC8KETDC		3	0	9	2	243	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - O/H/O - 1 2 - C/C4 - 1   7 - CO/C/H - 1 3 - C/C2/H2 - 1   8 - OI - 2 4 - C/C2/CO/O - 1   9 - GAUCHE - 3 5 - O/C/O - 1   10 - DUM1 - 2 Hf S Cp 300 400 500 600 800 1000 1500 -95.28 123.74 54.30 67.44 79.44 90.09 106.10 117.27 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 243
	IC8KETDD		3	0	9	2	81	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - C/C/H2/OO - 1 2 - C/C4 - 1   7 - OO/C/H - 1 3 - C/C2/H2 - 1   8 - OI - 2 4 - C/C2/CO/H - 1   9 - GAUCHE - 3 5 - CO/C/H - 1 Hf S Cp 300 400 500 600 800 1000 1500 -93.22 127.71 53.34 65.70 77.23 87.54 103.28 114.34 .00 CPINF = 148.03 NROTORS: 9 SYMMETRY 81
<b>ROH, OOROH, HOOROH</b>	BC8H16OH-C		3	1	8	1	1458	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   6 - GAUCHE - 3 2 - C/C4 - 1   7 - H15 - 1 3 - C/C2/H/O - 1   8 - OI - 1 4 - O/C/H - 1   9 - T - 1 5 - C/C3/H - 1 Hf S Cp 300 400 500 600 800 1000 1500 -48.86 114.95 47.57 59.29 70.42 80.23 95.89 106.78 .00 CPINF = 143.06 NROTORS: 8 SYMMETRY 1458

			Gauche	H15	Rotors	OI	Symm.	THERM groups
BC8H16OH-CO2		3	1	10	2	729	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   6 - GAUCHE - 3 2 - C/C4 - 1   7 - H15 - 1 3 - O/C/H - 1   8 - C/C2/H/O - 1 4 - C/C3/OO - 1   9 - OO/C/H - 1 5 - OI - 2   10 - ALPEROX - 1 Hf S Cp 300 400 500 600 800 1000 1500 -87.07 125.25 56.16 69.55 81.35 91.40 107.04 117.82 .00 CPINF = 153.00 NROTORS:10 SYMMETRY 243	
BC8H16O-CO2H		3	1	10	2	729	UNITS:KCAL GROUPS 11 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   7 - OI - 2 2 - C/C4 - 1   8 - GAUCHE - 3 3 - C/C2/H/O - 1   9 - H15 - 1 4 - O/C/H - 1   10 - DUM1 - 2 5 - C/C3/OO - 1   11 - ALKOXY - 1 6 - OO/C/H - 1 Hf S Cp 300 400 500 600 800 1000 1500 -65.42 121.83 57.85 70.73 82.52 92.58 108.16 118.89 .00 CPINF = 153.00 NROTORS:10 SYMMETRY 729	
CC8H16OH-B		3	1	8	0	729	UNITS:KCAL GROUPS 8 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   5 - O/C/H - 1 2 - C/C4 - 1   6 - GAUCHE - 3 3 - C/C2/H2 - 1   7 - H15 - 1 4 - C/C3/O - 1   8 - S - 1 Hf S Cp 300 400 500 600 800 1000 1500 -49.78 113.80 47.75 59.21 70.36 80.29 96.36 107.57 129.66 CPINF = 143.06 NROTORS: 8 SYMMETRY 729	
CC8H16OH-BO2		3	1	10	2	729	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   6 - O/C/H - 1 2 - C/C4 - 1   7 - H15 - 1 3 - C/C2/H/OO - 1   8 - GAUCHE - 3 4 - OO/C/H - 1   9 - OI - 2 5 - C/C3/O - 1   10 - ALPEROX - 1 Hf S Cp 300 400 500 600 800 1000 1500 -85.21 125.33 56.72 69.70 81.33 91.59 107.62 118.71 .00 CPINF = 153.00 NROTORS:10 SYMMETRY 729	

			Gauche	H15	Rotors	OI	Symm.	THERM groups
CC8H16O-BO2H		3	1	10	2	729	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   6 - O/C/H - 1 2 - C/C4 - 1   7 - H15 - 1 3 - C/C2/H/OO - 1   8 - GAUCHE - 3 4 - OO/C/H - 1   9 - OI - 2 5 - C/C3/O - 1   10 - ALKOXY - 1 Hf S Cp 300 400 500 600 800 1000 1500 -65.56 124.10 58.41 70.88 82.50 92.77 108.74 119.78 .00 CPINF = 153.00 NROTORS:10 SYMMETRY 729	
CC8H16OH-D		2	1	9	1	486	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   6 - OI - 1 2 - C/C4 - 1   7 - GAUCHE - 3 3 - C/C2/H2 - 1   8 - H15 - 1 4 - C/C3/O - 1   9 - P - 1 5 - O/C/H - 1 Hf S Cp 300 400 500 600 800 1000 1500 -46.70 114.23 48.39 60.55 71.71 81.50 97.44 108.46 130.37 CPINF = 142.07 NROTORS: 9 SYMMETRY 486	
CC8H16OH-DO2		3	0	10	2	243	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - C/C/H2/OO - 1 2 - C/C4 - 1   7 - OO/C/H - 1 3 - C/C2/H2 - 1   8 - OI - 2 4 - C/C3/O - 1   9 - GAUCHE - 3 5 - O/C/H - 1   10 - ALPEROX - 1 Hf S Cp 300 400 500 600 800 1000 1500 -82.69 128.96 55.51 68.56 80.41 90.72 107.35 118.78 .00 CPINF = 153.00 NROTORS:10 SYMMETRY 243	
CC8H16O-DO2H		3	0	10	2	243	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - C/C/H2/OO - 1 2 - C/C4 - 1   7 - OO/C/H - 1 3 - C/C2/H2 - 1   8 - OI - 2 4 - C/C3/O - 1   9 - GAUCHE - 3 5 - O/C/H - 1   10 - ALKOXY - 1 Hf S Cp 300 400 500 600 800 1000 1500 -63.04 127.73 57.20 69.74 81.58 91.90 108.47 119.85 .00 CPINF = 153.00 NROTORS:10 SYMMETRY 243	

			Gauche	H15	Rotors	OI	Symm.	THERM groups
	DC8H16OH-C		3	0	8	1	243	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - O/C/H - 1 2 - C/C4 - 1   7 - OI - 1 3 - C/C2/H2 - 1   8 - GAUCHE - 3 4 - C/C3/H - 1   9 - T - 1 5 - C/C/H2/O - 1 Hf S Cp 300 400 500 600 800 1000 1500 -46.33 119.59 46.88 58.54 69.78 79.74 95.75 106.96 .00 CPINF = 143.06 NROTORS: 8 SYMMETRY 243
	DC8H16OH-CO2		3	0	10	2	243	UNITS:KCAL GROUPS 11 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   7 - O/C/H - 1 2 - C/C4 - 1   8 - OI - 2 3 - C/C2/H2 - 1   9 - GAUCHE - 3 4 - C/C3/OO - 1   10 - DUM1 - 2 5 - OO/C/H - 1   11 - ALKOXY - 1 6 - C/C/H2/O - 1 Hf S Cp 300 400 500 600 800 1000 1500 -62.89 125.10 57.16 69.98 81.88 92.09 108.02 119.07 .00 CPINF = 153.00 NROTORS:10 SYMMETRY 243
	DC8H16O-CO2H		3	1	10	2	243	UNITS:KCAL GROUPS 11 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   7 - O/C/H - 1 2 - C/C4 - 1   8 - OI - 2 3 - C/C2/H2 - 1   9 - GAUCHE - 3 4 - C/C3/OO - 1   10 - DUM1 - 2 5 - OO/C/H - 1   11 - ALKOXY - 1 6 - C/C/H2/O - 1 Hf S Cp 300 400 500 600 800 1000 1500 -62.89 125.10 57.16 69.98 81.88 92.09 108.02 119.07 .00 CPINF = 153.00 NROTORS:10 SYMMETRY 243
<b>P(OOH)2</b>	AC8H15(OOH)AA		2	0	11	2	18	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - OO/C/H - 2 2 - C/C3/H - 1   7 - GAUCHE - 2 3 - C/C2/H2 - 1   8 - OI - 2 4 - C/C4 - 1   9 - P - 1 5 - C/C/H2/OO - 2 Hf S Cp 300 400 500 600 800 1000 1500 -43.61 144.08 58.79 72.86 85.28 95.90 112.18 123.46 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 18

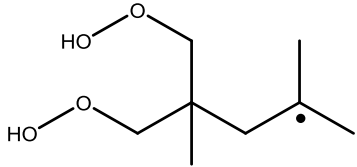
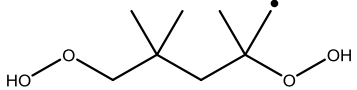
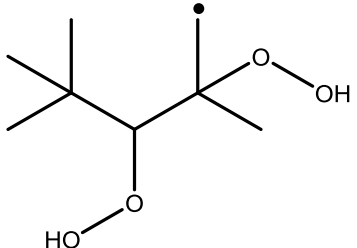
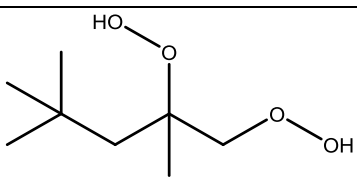
			Gauche	H15	Rotors	OI	Symm.	THERM groups
AC8H15(OOH)AB		2	0	11	4	54	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - C/C/H2/OO - 1 2 - C/C3/H - 1   7 - OI - 4 3 - C/C2/H/OO - 1   8 - GAUCHE - 2 4 - OO/C/H - 2   9 - P - 1 5 - C/C4 - 1 Hf S Cp 300 400 500 600 800 1000 1500 -47.63 143.19 60.00 74.00 86.20 96.77 112.45 123.39 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 54	
AC8H15(OOH)AC		2	0	11	3	54	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - C/C2/H2 - 1 2 - C/C3/OO - 1   7 - C/C4 - 1 3 - OO/C/H - 2   8 - C/C/H2/OO - 1 4 - OI - 3   9 - DUM1 - 2 5 - GAUCHE - 2   10 - P - 1 Hf S Cp 300 400 500 600 800 1000 1500 -49.96 139.69 59.82 73.63 85.74 96.15 112.14 123.29 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 54	
AC8H15(OOH)AD		2	0	11	4	18	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - C/C4 - 1 2 - C/C3/H - 1   7 - GAUCHE - 2 3 - C/C/H2/OO - 2   8 - OI - 4 4 - OO/C/H - 2   9 - P - 1 5 - C/C2/H2 - 1 Hf S Cp 300 400 500 600 800 1000 1500 -43.61 146.82 58.79 72.86 85.28 95.90 112.18 123.46 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 18	
AC8H15(OOH)BC		2	1	11	3	162	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 5   6 - OI - 3 2 - C/C4 - 1   7 - GAUCHE - 2 3 - C/C2/H/OO - 1   8 - H15 - 1 4 - OO/C/H - 2   9 - DUM1 - 2 5 - C/C3/OO - 1   10 - P - 1 Hf S Cp 300 400 500 600 800 1000 1500 -52.48 136.07 61.03 74.77 86.66 97.02 112.41 123.22 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 162	

			Gauche	H15	Rotors	OI	Symm.	THERM groups
AC8H15(OOH)BD		2	0	11	4	54	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - C/C4 - 1 2 - C/C3/H - 1   7 - GAUCHE - 2 3 - C/C/H2/OO - 1   8 - OI - 4 4 - OO/C/H - 2   9 - P - 1 5 - C/C2/H/OO - 1 Hf S Cp 300 400 500 600 800 1000 1500 -47.63 143.19 60.00 74.00 86.20 96.77 112.45 123.39 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 54	
AC8H15(OOH)CD		2	0	11	3	54	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - OI - 3   6 - C/C3/OO - 1 2 - GAUCHE - 2   7 - OO/C/H - 2 3 - C/C/H3 - 4   8 - C/C/H2/OO - 1 4 - C/C4 - 1   9 - P - 1 5 - C/C2/H2 - 1 Hf S Cp 300 400 500 600 800 1000 1500 -51.96 139.69 59.82 73.63 85.74 96.15 112.14 123.29 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 54	
AC8H15(OOH)DD		2	0	11	2	18	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - GAUCHE - 2   6 - C/C3/H - 1 2 - OI - 2   7 - C/C/H2/OO - 2 3 - C/C4 - 1   8 - OO/C/H - 2 4 - C/C/H3 - 3   9 - P - 1 5 - C/C2/H2 - 1 Hf S Cp 300 400 500 600 800 1000 1500 -43.61 144.08 58.79 72.86 85.28 95.90 112.18 123.46 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 18	
BC8H15(OOH)2AC		3	0	11	2	81	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - C/C3/OO - 1 2 - C/C4 - 1   7 - OI - 2 3 - OO/C/H - 2   8 - GAUCHE - 3 4 - C/C/H2/OO - 1   9 - DUM1 - 2 5 - C/C2/H2 - 1   10 - S - 1 Hf S Cp 300 400 500 600 800 1000 1500 -52.24 139.27 59.18 72.29 84.39 94.94 111.06 122.40 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 81	

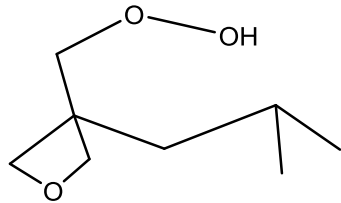
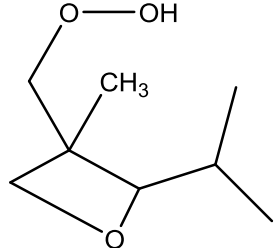
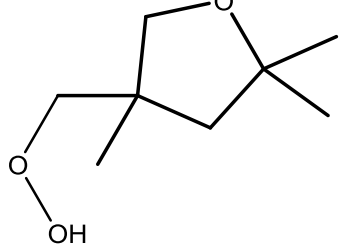
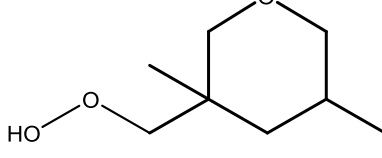
			Gauche	H15	Rotors	OI	Symm.	THERM groups
BC8H15(OOH)2CD		3	0	11	3	243	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C4 - 1   6 - C/C/H2/OO - 1 2 - C/C/H3 - 4   7 - OI - 3 3 - C/C2/H2 - 1   8 - GAUCHE - 3 4 - C/C3/OO - 1   9 - DUM1 - 2 5 - OO/C/H - 2   10 - S - 1 Hf S Cp 300 400 500 600 800 1000 1500 -52.24 138.46 59.18 72.29 84.39 94.94 111.06 122.40 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 243	
BC8H15(OOH)AA		3	0	11	2	27	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - OO/C/H - 2 2 - C/C3/H - 1   7 - OI - 2 3 - C/C2/H2 - 1   8 - GAUCHE - 3 4 - C/C4 - 1   9 - S - 1 5 - C/C/H2/OO - 2 Hf S Cp 300 400 500 600 800 1000 1500 -45.89 145.02 58.15 71.52 83.93 94.69 111.10 122.57 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 27	
BC8H15(OOH)AD		3	0	11	3	27	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - C/C4 - 1 2 - C/C3/H - 1   7 - OI - 3 3 - C/C/H2/OO - 2   8 - GAUCHE - 3 4 - OO/C/H - 2   9 - S - 1 5 - C/C2/H2 - 1 Hf S Cp 300 400 500 600 800 1000 1500 -45.89 146.39 58.15 71.52 83.93 94.69 111.10 122.57 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 27	
BC8H15(OOH)DD		3	0	11		81	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - OO/C/H - 2 2 - C/C4 - 1   7 - OI - 2 3 - C/C2/H2 - 1   8 - GAUCHE - 3 4 - C/C3/H - 1   9 - S - 1 5 - C/C/H2/OO - 2 Hf S Cp 300 400 500 600 800 1000 1500 -45.89 142.84 58.15 71.52 83.93 94.69 111.10 122.57 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 81	

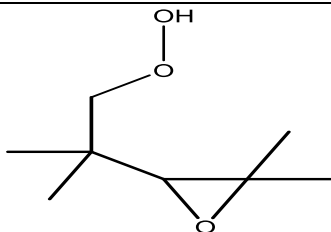
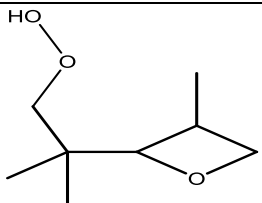
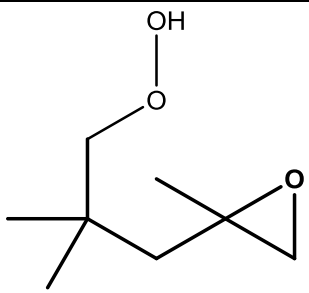
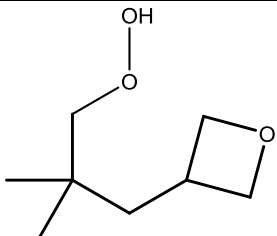
			Gauche	H15	Rotors	OI	Symm.	THERM groups
CC8H15(OOH)2AB		3	0	11	3	162	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C4 - 1   6 - C/C3/H - 1 2 - C/C/H3 - 4   7 - OI - 3 3 - C/C/H2/OO - 1   8 - GAUCHE - 3 4 - OO/C/H - 2   9 - T - 1 5 - C/C2/H/OO - 1 Hf S Cp 300 400 500 600 800 1000 1500 -51.46 142.68 59.56 72.52 84.43 95.07 111.17 122.50 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 162	
CC8H15(OOH)2AD		3	0	11	2	27	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C4 - 1   6 - C/C3/H - 1 2 - C/C/H3 - 3   7 - OI - 2 3 - C/C/H2/OO - 2   8 - GAUCHE - 3 4 - OO/C/H - 2   9 - T - 1 5 - C/C2/H2 - 1 Hf S Cp 300 400 500 600 800 1000 1500 -47.44 146.31 58.35 71.38 83.51 94.20 110.90 122.57 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 27	
CC8H15(OOH)2BD		3	0	11	3	243	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - C/C/H2/OO - 1 2 - C/C4 - 1   7 - GAUCHE - 3 3 - C/C2/H/OO - 1   8 - OI - 3 4 - OO/C/H - 2   9 - T - 1 5 - C/C3/H - 1 Hf S Cp 300 400 500 600 800 1000 1500 -51.46 141.88 59.56 72.52 84.43 95.07 111.17 122.50 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 243	
CC8H15(OOH)2DD		3	0	11	2	162	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C4 - 1   6 - OO/C/H - 2 2 - C/C/H3 - 3   7 - OI - 2 3 - C/C2/H2 - 1   8 - GAUCHE - 3 4 - C/C3/H - 1   9 - T - 1 5 - C/C/H2/OO - 2 Hf S Cp 300 400 500 600 800 1000 1500 -47.44 142.75 58.35 71.38 83.51 94.20 110.90 122.57 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 162	

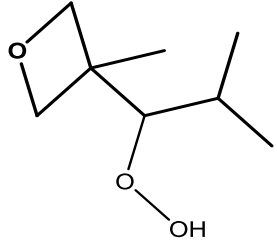
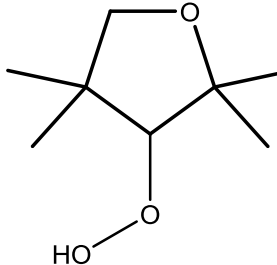
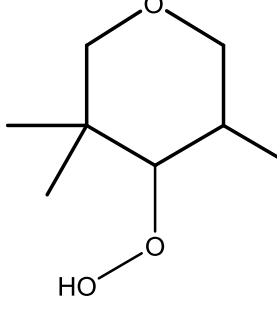
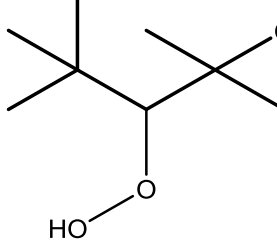


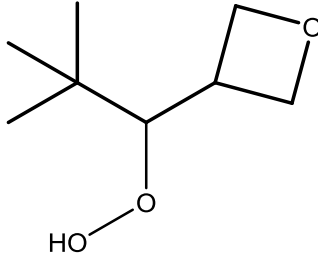
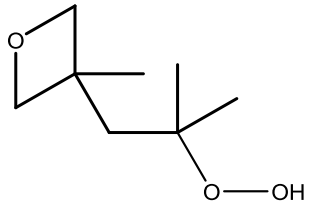
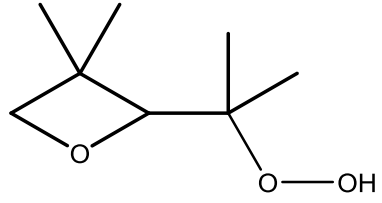
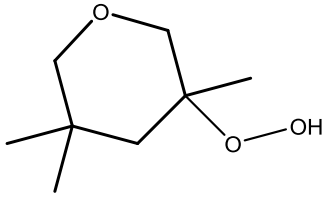
			Gauche	H15	Rotors	OI	Symm.	THERM groups
CC8H15(OOH)AA		3	0	11	2	54	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C4 - 1   6 - OO/C/H - 2 2 - C/C/H3 - 3   7 - OI - 2 3 - C/C3/H - 1   8 - GAUCHE - 3 4 - C/C2/H2 - 1   9 - T - 1 5 - C/C/H2/OO - 2 Hf S Cp 300 400 500 600 800 1000 1500 -47.44 144.93 58.35 71.38 83.51 94.20 110.90 122.57 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 54	
DC8H15(OOH)2AC		2	0	11	3	54	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - C/C3/OO - 1 2 - C/C4 - 1   7 - OI - 3 3 - C/C/H2/OO - 1   8 - GAUCHE - 2 4 - OO/C/H - 2   9 - DUM1 - 2 5 - C/C2/H2 - 1   10 - P - 1 Hf S Cp 300 400 500 600 800 1000 1500 -49.96 139.69 59.82 73.63 85.74 96.15 112.14 123.29 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 54	
DC8H15(OOH)2BC		2	1	11	4	486	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C4 - 1   6 - OI - 4 2 - C/C/H3 - 5   7 - GAUCHE - 2 3 - C/C2/H/OO - 1   8 - H15 - 1 4 - OO/C/H - 2   9 - DUM1 - 2 5 - C/C3/OO - 1   10 - P - 1 Hf S Cp 300 400 500 600 800 1000 1500 -52.48 135.26 61.03 74.77 86.66 97.02 112.41 123.22 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 486	
DC8H15(OOH)2CD		2	0	11	3	162	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - GAUCHE - 2 2 - C/C4 - 1   7 - C/C/H2/OO - 1 3 - C/C3/OO - 1   8 - C/C2/H2 - 1 4 - OO/C/H - 2   9 - DUM1 - 2 5 - OI - 3   10 - P - 1 Hf S Cp 300 400 500 600 800 1000 1500 -49.96 137.51 59.82 73.63 85.74 96.15 112.14 123.29 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 162	

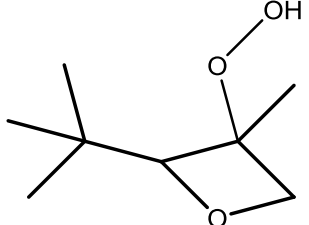
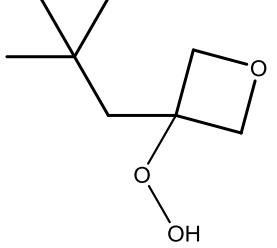
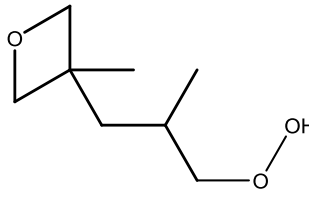
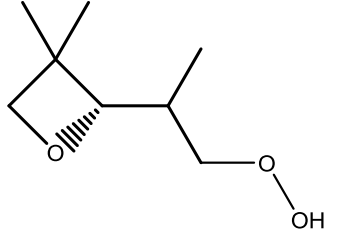
			Gauche	H15	Rotors	OI	Symm.	THERM groups
DC8H15(OOH)AA		2	0	11	3	18	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - GAUCHE - 2   6 - OO/C/H - 2 2 - OI - 3   7 - C/C/H2/OO - 2 3 - C/C/H3 - 3   8 - C/C4 - 1 4 - C/C3/H - 1   9 - P - 1 5 - C/C2/H2 - 1 Hf S Cp 300 400 500 600 800 1000 1500 -43.61 145.45 58.79 72.86 85.28 95.90 112.18 123.46 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 18	
DC8H15(OOH)AB		2	0	11	4	54	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - C/C/H2/OO - 1 2 - C/C3/H - 1   7 - OI - 4 3 - C/C2/H/OO - 1   8 - GAUCHE - 2 4 - OO/C/H - 2   9 - P - 1 5 - C/C4 - 1 Hf S Cp 300 400 500 600 800 1000 1500 -47.63 143.19 60.00 74.00 86.20 96.77 112.45 123.39 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 54	
DC8H15(OOH)AD		2	0	11	3	18	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - C/C4 - 1 2 - C/C3/H - 1   7 - GAUCHE - 2 3 - C/C/H2/OO - 2   8 - OI - 3 4 - OO/C/H - 2   9 - P - 1 5 - C/C2/H2 - 1 Hf S Cp 300 400 500 600 800 1000 1500 -43.61 145.45 58.79 72.86 85.28 95.90 112.18 123.46 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 18	
DC8H15(OOH)BD		2	0	11	4	162	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - C/C4 - 1 2 - C/C3/H - 1   7 - OI - 4 3 - C/C/H2/OO - 1   8 - GAUCHE - 2 4 - OO/C/H - 2   9 - P - 1 5 - C/C2/H/OO - 1 Hf S Cp 300 400 500 600 800 1000 1500 -47.63 141.01 60.00 74.00 86.20 96.77 112.45 123.39 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 162	

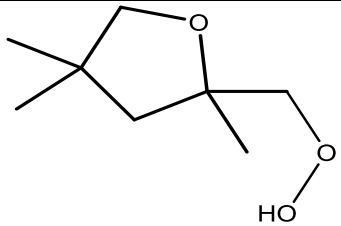
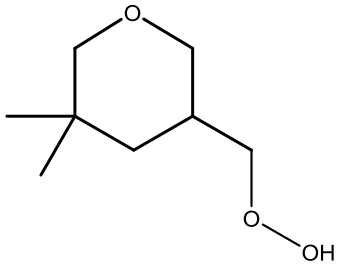
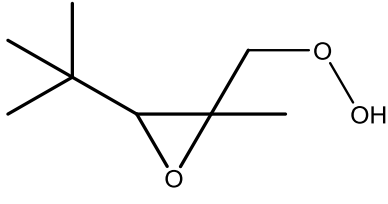
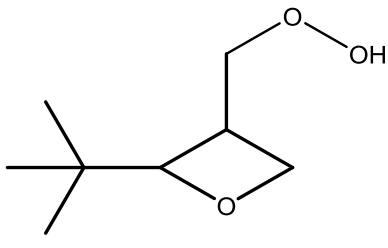
			Gauche	H15	Rotors	OI	Symm.	THERM groups																																																																																																			
HPCE	A(OOH)ETRAA		3	0	7	1	9	UNITS:KCAL GROUPS 12 <table border="0"> <tr> <td>Gr #</td><td>-</td><td>GROUP ID</td><td>-</td><td>Quantity</td><td></td><td>Gr #</td><td>-</td><td>GROUP ID</td><td>-</td><td>Quantity</td> </tr> <tr> <td>1</td><td>-</td><td>C/C/H3</td><td>-</td><td>2</td><td> </td><td>7</td><td>-</td><td>C/C/H2/O</td><td>-</td><td>2</td> </tr> <tr> <td>2</td><td>-</td><td>C/C3/H</td><td>-</td><td>1</td><td> </td><td>8</td><td>-</td><td>O/C2</td><td>-</td><td>1</td> </tr> <tr> <td>3</td><td>-</td><td>C/C2/H2</td><td>-</td><td>1</td><td> </td><td>9</td><td>-</td><td>CY/C3O</td><td>-</td><td>1</td> </tr> <tr> <td>4</td><td>-</td><td>C/C/H2/OO</td><td>-</td><td>1</td><td> </td><td>10</td><td>-</td><td>GAUCHE</td><td>-</td><td>3</td> </tr> <tr> <td>5</td><td>-</td><td>OO/C/H</td><td>-</td><td>1</td><td> </td><td>11</td><td>-</td><td>OI</td><td>-</td><td>1</td> </tr> <tr> <td>6</td><td>-</td><td>C/C4</td><td>-</td><td>1</td><td> </td><td>12</td><td>-</td><td>DUM2</td><td>-</td><td>4</td> </tr> </table> <table border="0"> <tr> <td>Hf</td><td>S</td><td>Cp</td><td>300</td><td>400</td><td>500</td><td>600</td><td>800</td><td>1000</td><td>1500</td><td></td> </tr> <tr> <td>-72.02</td><td>121.68</td><td>48.57</td><td>62.75</td><td>76.03</td><td>87.03</td><td>102.90</td><td>113.92</td><td></td><td></td><td>.00</td> </tr> </table> CPINF = 150.02 NROTORS: 7 SYMMETRY 9	Gr #	-	GROUP ID	-	Quantity		Gr #	-	GROUP ID	-	Quantity	1	-	C/C/H3	-	2		7	-	C/C/H2/O	-	2	2	-	C/C3/H	-	1		8	-	O/C2	-	1	3	-	C/C2/H2	-	1		9	-	CY/C3O	-	1	4	-	C/C/H2/OO	-	1		10	-	GAUCHE	-	3	5	-	OO/C/H	-	1		11	-	OI	-	1	6	-	C/C4	-	1		12	-	DUM2	-	4	Hf	S	Cp	300	400	500	600	800	1000	1500		-72.02	121.68	48.57	62.75	76.03	87.03	102.90	113.92			.00
Gr #	-	GROUP ID	-	Quantity		Gr #	-	GROUP ID	-	Quantity																																																																																																	
1	-	C/C/H3	-	2		7	-	C/C/H2/O	-	2																																																																																																	
2	-	C/C3/H	-	1		8	-	O/C2	-	1																																																																																																	
3	-	C/C2/H2	-	1		9	-	CY/C3O	-	1																																																																																																	
4	-	C/C/H2/OO	-	1		10	-	GAUCHE	-	3																																																																																																	
5	-	OO/C/H	-	1		11	-	OI	-	1																																																																																																	
6	-	C/C4	-	1		12	-	DUM2	-	4																																																																																																	
Hf	S	Cp	300	400	500	600	800	1000	1500																																																																																																		
-72.02	121.68	48.57	62.75	76.03	87.03	102.90	113.92			.00																																																																																																	
	A(OOH)ETRAB		3	0	7	3	27	UNITS:KCAL GROUPS 12 <table border="0"> <tr> <td>Gr #</td><td>-</td><td>GROUP ID</td><td>-</td><td>Quantity</td><td></td><td>Gr #</td><td>-</td><td>GROUP ID</td><td>-</td><td>Quantity</td> </tr> <tr> <td>1</td><td>-</td><td>C/C/H3</td><td>-</td><td>3</td><td> </td><td>7</td><td>-</td><td>C/C/H2/OO</td><td>-</td><td>1</td> </tr> <tr> <td>2</td><td>-</td><td>C/C3/H</td><td>-</td><td>1</td><td> </td><td>8</td><td>-</td><td>OO/C/H</td><td>-</td><td>1</td> </tr> <tr> <td>3</td><td>-</td><td>C/C2/H/O</td><td>-</td><td>1</td><td> </td><td>9</td><td>-</td><td>CY/C3O</td><td>-</td><td>1</td> </tr> <tr> <td>4</td><td>-</td><td>O/C2</td><td>-</td><td>1</td><td> </td><td>10</td><td>-</td><td>GAUCHE</td><td>-</td><td>3</td> </tr> <tr> <td>5</td><td>-</td><td>C/C/H2/O</td><td>-</td><td>1</td><td> </td><td>11</td><td>-</td><td>OI</td><td>-</td><td>3</td> </tr> <tr> <td>6</td><td>-</td><td>C/C4</td><td>-</td><td>1</td><td> </td><td>12</td><td>-</td><td>DUM2</td><td>-</td><td>4</td> </tr> </table> <table border="0"> <tr> <td>Hf</td><td>S</td><td>Cp</td><td>300</td><td>400</td><td>500</td><td>600</td><td>800</td><td>1000</td><td>1500</td><td></td> </tr> <tr> <td>-76.05</td><td>121.16</td><td>49.26</td><td>63.50</td><td>76.67</td><td>87.52</td><td>103.04</td><td>113.74</td><td></td><td></td><td>.00</td> </tr> </table> CPINF = 150.02 NROTORS: 7 SYMMETRY 27	Gr #	-	GROUP ID	-	Quantity		Gr #	-	GROUP ID	-	Quantity	1	-	C/C/H3	-	3		7	-	C/C/H2/OO	-	1	2	-	C/C3/H	-	1		8	-	OO/C/H	-	1	3	-	C/C2/H/O	-	1		9	-	CY/C3O	-	1	4	-	O/C2	-	1		10	-	GAUCHE	-	3	5	-	C/C/H2/O	-	1		11	-	OI	-	3	6	-	C/C4	-	1		12	-	DUM2	-	4	Hf	S	Cp	300	400	500	600	800	1000	1500		-76.05	121.16	49.26	63.50	76.67	87.52	103.04	113.74			.00
Gr #	-	GROUP ID	-	Quantity		Gr #	-	GROUP ID	-	Quantity																																																																																																	
1	-	C/C/H3	-	3		7	-	C/C/H2/OO	-	1																																																																																																	
2	-	C/C3/H	-	1		8	-	OO/C/H	-	1																																																																																																	
3	-	C/C2/H/O	-	1		9	-	CY/C3O	-	1																																																																																																	
4	-	O/C2	-	1		10	-	GAUCHE	-	3																																																																																																	
5	-	C/C/H2/O	-	1		11	-	OI	-	3																																																																																																	
6	-	C/C4	-	1		12	-	DUM2	-	4																																																																																																	
Hf	S	Cp	300	400	500	600	800	1000	1500																																																																																																		
-76.05	121.16	49.26	63.50	76.67	87.52	103.04	113.74			.00																																																																																																	
	A(OOH)ETRAC		2	0	6	2	27	UNITS:KCAL GROUPS 11 <table border="0"> <tr> <td>Gr #</td><td>-</td><td>GROUP ID</td><td>-</td><td>Quantity</td><td></td><td>Gr #</td><td>-</td><td>GROUP ID</td><td>-</td><td>Quantity</td> </tr> <tr> <td>1</td><td>-</td><td>GAUCHE</td><td>-</td><td>2</td><td> </td><td>7</td><td>-</td><td>C/C2/H2</td><td>-</td><td>1</td> </tr> <tr> <td>2</td><td>-</td><td>C/C/H3</td><td>-</td><td>3</td><td> </td><td>8</td><td>-</td><td>CY/C4O</td><td>-</td><td>1</td> </tr> <tr> <td>3</td><td>-</td><td>C/C3/O</td><td>-</td><td>1</td><td> </td><td>9</td><td>-</td><td>C/C/H2/OO</td><td>-</td><td>1</td> </tr> <tr> <td>4</td><td>-</td><td>O/C2</td><td>-</td><td>1</td><td> </td><td>10</td><td>-</td><td>OO/C/H</td><td>-</td><td>1</td> </tr> <tr> <td>5</td><td>-</td><td>C/C/H2/O</td><td>-</td><td>1</td><td> </td><td>11</td><td>-</td><td>OI</td><td>-</td><td>2</td> </tr> <tr> <td>6</td><td>-</td><td>C/C4</td><td>-</td><td>1</td><td> </td><td></td><td></td><td></td><td></td><td></td> </tr> </table> <table border="0"> <tr> <td>Hf</td><td>S</td><td>Cp</td><td>300</td><td>400</td><td>500</td><td>600</td><td>800</td><td>1000</td><td>1500</td><td></td> </tr> <tr> <td>-95.35</td><td>117.90</td><td>47.79</td><td>61.85</td><td>75.16</td><td>86.39</td><td>103.07</td><td>114.57</td><td></td><td></td><td>.00</td> </tr> </table> CPINF = 151.01 NROTORS: 6 SYMMETRY 27	Gr #	-	GROUP ID	-	Quantity		Gr #	-	GROUP ID	-	Quantity	1	-	GAUCHE	-	2		7	-	C/C2/H2	-	1	2	-	C/C/H3	-	3		8	-	CY/C4O	-	1	3	-	C/C3/O	-	1		9	-	C/C/H2/OO	-	1	4	-	O/C2	-	1		10	-	OO/C/H	-	1	5	-	C/C/H2/O	-	1		11	-	OI	-	2	6	-	C/C4	-	1							Hf	S	Cp	300	400	500	600	800	1000	1500		-95.35	117.90	47.79	61.85	75.16	86.39	103.07	114.57			.00
Gr #	-	GROUP ID	-	Quantity		Gr #	-	GROUP ID	-	Quantity																																																																																																	
1	-	GAUCHE	-	2		7	-	C/C2/H2	-	1																																																																																																	
2	-	C/C/H3	-	3		8	-	CY/C4O	-	1																																																																																																	
3	-	C/C3/O	-	1		9	-	C/C/H2/OO	-	1																																																																																																	
4	-	O/C2	-	1		10	-	OO/C/H	-	1																																																																																																	
5	-	C/C/H2/O	-	1		11	-	OI	-	2																																																																																																	
6	-	C/C4	-	1																																																																																																							
Hf	S	Cp	300	400	500	600	800	1000	1500																																																																																																		
-95.35	117.90	47.79	61.85	75.16	86.39	103.07	114.57			.00																																																																																																	
	A(OOH)ETRAD		1	0	5	3	9	UNITS:KCAL GROUPS 10 <table border="0"> <tr> <td>Gr #</td><td>-</td><td>GROUP ID</td><td>-</td><td>Quantity</td><td></td><td>Gr #</td><td>-</td><td>GROUP ID</td><td>-</td><td>Quantity</td> </tr> <tr> <td>1</td><td>-</td><td>C/C/H3</td><td>-</td><td>2</td><td> </td><td>6</td><td>-</td><td>CY/C5O</td><td>-</td><td>1</td> </tr> <tr> <td>2</td><td>-</td><td>C/C3/H</td><td>-</td><td>1</td><td> </td><td>7</td><td>-</td><td>C/C/H2/OO</td><td>-</td><td>1</td> </tr> <tr> <td>3</td><td>-</td><td>C/C/H2/O</td><td>-</td><td>2</td><td> </td><td>8</td><td>-</td><td>OO/C/H</td><td>-</td><td>1</td> </tr> <tr> <td>4</td><td>-</td><td>O/C2</td><td>-</td><td>1</td><td> </td><td>9</td><td>-</td><td>OI</td><td>-</td><td>3</td> </tr> <tr> <td>5</td><td>-</td><td>C/C4</td><td>-</td><td>1</td><td> </td><td>10</td><td>-</td><td>GAUCHE</td><td>-</td><td>1</td> </tr> </table> <table border="0"> <tr> <td>Hf</td><td>S</td><td>Cp</td><td>300</td><td>400</td><td>500</td><td>600</td><td>800</td><td>1000</td><td>1500</td><td></td> </tr> <tr> <td>-88.91</td><td>103.40</td><td>41.04</td><td>54.47</td><td>67.06</td><td>77.54</td><td>92.56</td><td>102.86</td><td></td><td></td><td>.00</td> </tr> </table> CPINF = 152.01 NROTORS: 5 SYMMETRY 9	Gr #	-	GROUP ID	-	Quantity		Gr #	-	GROUP ID	-	Quantity	1	-	C/C/H3	-	2		6	-	CY/C5O	-	1	2	-	C/C3/H	-	1		7	-	C/C/H2/OO	-	1	3	-	C/C/H2/O	-	2		8	-	OO/C/H	-	1	4	-	O/C2	-	1		9	-	OI	-	3	5	-	C/C4	-	1		10	-	GAUCHE	-	1	Hf	S	Cp	300	400	500	600	800	1000	1500		-88.91	103.40	41.04	54.47	67.06	77.54	92.56	102.86			.00											
Gr #	-	GROUP ID	-	Quantity		Gr #	-	GROUP ID	-	Quantity																																																																																																	
1	-	C/C/H3	-	2		6	-	CY/C5O	-	1																																																																																																	
2	-	C/C3/H	-	1		7	-	C/C/H2/OO	-	1																																																																																																	
3	-	C/C/H2/O	-	2		8	-	OO/C/H	-	1																																																																																																	
4	-	O/C2	-	1		9	-	OI	-	3																																																																																																	
5	-	C/C4	-	1		10	-	GAUCHE	-	1																																																																																																	
Hf	S	Cp	300	400	500	600	800	1000	1500																																																																																																		
-88.91	103.40	41.04	54.47	67.06	77.54	92.56	102.86			.00																																																																																																	

			Gauche	H15	Rotors	OI	Symm.	THERM groups
A(OOH)ETRBC		3	0	8	2	81	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - O/C2 - 1 2 - C/C4 - 1   7 - C/C3/O - 1 3 - C/C/H2/OO - 1   8 - GAUCHE - 3 4 - OO/C/H - 1   9 - CY/C2O - 1 5 - C/C2/H/O - 1   10 - OI - 2 Hf S Cp 300 400 500 600 800 1000 1500 -76.81 119.20 52.33 65.65 78.07 88.49 103.85 114.45 .00 CPINF = 149.02 NROTORS: 8 SYMMETRY 81	
A(OOH)ETRBD		3	0	7	3	27	UNITS:KCAL GROUPS 12 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   7 - C/C/H2/OO - 1 2 - C/C3/H - 1   8 - CY/C3O - 1 3 - C/C/H2/O - 1   9 - OO/C/H - 1 4 - O/C2 - 1   10 - GAUCHE - 3 5 - C/C2/H/O - 1   11 - OI - 3 6 - C/C4 - 1   12 - DUM2 - 4 Hf S Cp 300 400 500 600 800 1000 1500 -76.05 121.16 49.26 63.50 76.67 87.52 103.04 113.74 .00 CPINF = 150.02 NROTORS: 7 SYMMETRY 27	
A(OOH)ETRC D		3	0	8	1	27	UNITS:KCAL GROUPS 11 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   7 - C/C/H2/O - 1 2 - C/C4 - 1   8 - O/C2 - 1 3 - C/C/H2/OO - 1   9 - CY/C2O - 1 4 - OO/C/H - 1   10 - OI - 1 5 - C/C2/H2 - 1   11 - GAUCHE - 3 6 - C/C3/O - 1 Hf S Cp 300 400 500 600 800 1000 1500 -72.78 121.09 51.64 64.90 77.43 88.00 103.71 114.63 .00 CPINF = 149.02 NROTORS: 8 SYMMETRY 27	
A(OOH)ETRDD		3	0	7	1	9	UNITS:KCAL GROUPS 12 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 2   7 - C/C/H2/O - 2 2 - C/C4 - 1   8 - O/C2 - 1 3 - C/C/H2/OO - 1   9 - CY/C3O - 1 4 - OO/C/H - 1   10 - GAUCHE - 3 5 - C/C2/H2 - 1   11 - OI - 1 6 - C/C3/H - 1   12 - DUM2 - 4 Hf S Cp 300 400 500 600 800 1000 1500 -72.02 121.68 48.57 62.75 76.03 87.03 102.90 113.92 .00 CPINF = 150.02	

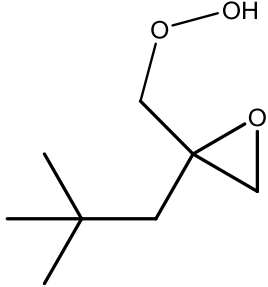
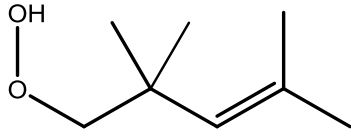
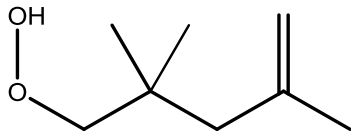
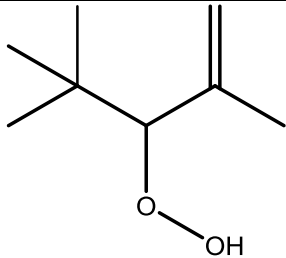
			Gauche	H15	Rotors	OI	Symm.	THERM groups
								NROTORS: 7 SYMMETRY 9
B(OOH)ETRAA		3	0	7	2	27		UNITS:KCAL GROUPS 11 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   7 - O/C2 - 1 2 - C/C3/H - 1   8 - CY/C3O - 1 3 - C/C2/H/OO - 1   9 - GAUCHE - 3 4 - OO/C/H - 1   10 - OI - 2 5 - C/C4 - 1   11 - DUM2 - 4 6 - C/C/H2/O - 2 Hf S Cp 300 400 500 600 800 1000 1500 -76.04 119.43 49.78 63.89 76.95 87.90 103.17 113.85 .00 CPINF = 150.02 NROTORS: 7 SYMMETRY 27
B(OOH)ETRAC		2	0	6	2	81		UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - C/C2/H/OO - 1 2 - C/C4 - 1   7 - OO/C/H - 1 3 - C/C/H2/O - 1   8 - CY/C4O - 1 4 - O/C2 - 1   9 - OI - 2 5 - C/C3/O - 1   10 - GAUCHE - 2 Hf S Cp 300 400 500 600 800 1000 1500 -99.37 114.28 49.00 62.99 76.08 87.26 103.34 114.50 .00 CPINF = 151.01 NROTORS: 6 SYMMETRY 81
B(OOH)ETRAD		1	0	5	3	27		UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - O/C2 - 1 2 - C/C3/H - 1   7 - C/C4 - 1 3 - C/C2/H/OO - 1   8 - CY/C5O - 1 4 - OO/C/H - 1   9 - GAUCHE - 1 5 - C/C/H2/O - 2   10 - OI - 3 Hf S Cp 300 400 500 600 800 1000 1500 -97.93 109.43 47.84 62.69 76.41 87.94 104.06 115.27 .00 CPINF = 152.01 NROTORS: 5 SYMMETRY 27
B(OOH)ETRC D		3	0	8	3	243		UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - GAUCHE - 3 2 - C/C4 - 1   7 - OI - 3 3 - C/C2/H/OO - 1   8 - O/C2 - 1 4 - OO/C/H - 1   9 - C/C/H2/O - 1 5 - C/C3/O - 1   10 - CY/C2O - 1 Hf S Cp 300 400 500 600 800 1000 1500 -76.80 118.02 52.85 66.04 78.35 88.87 103.98 114.56 .00 CPINF = 149.02 NROTORS: 8

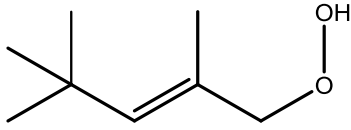
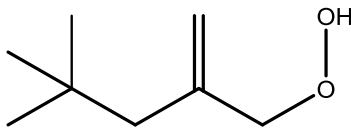
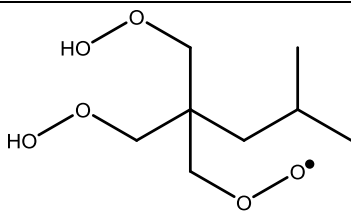
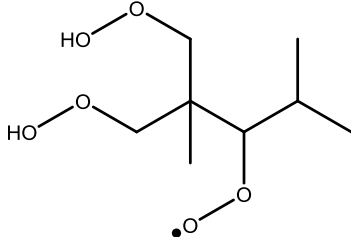
			Gauche	H15	Rotors	OI	Symm.	THERM groups
								SYMMETRY 243
B(OOH)ETRDD		3	0	7	2	81	UNITS:KCAL GROUPS 11 Gr # - GROUP ID - Quantity   Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   7 - O/C2 - 1 2 - C/C4 - 1   8 - CY/C3O - 1 3 - C/C2/H/OO - 1   9 - GAUCHE - 3 4 - OO/C/H - 1   10 - OI - 2 5 - C/C3/H - 1   11 - DUM2 - 4 6 - C/C/H2/O - 2 Hf S Cp 300 400 500 600 800 1000 1500 -76.04 117.25 49.78 63.89 76.95 87.90 103.17 113.85 .00 CPINF = 150.02 NROTORS: 7 SYMMETRY 81	
C(OOH)ETRAA		3	0	7	1	27	UNITS:KCAL GROUPS 12 Gr # - GROUP ID - Quantity   Gr # - GROUP ID - Quantity 1 - OI - 1   7 - C/C/H2/O - 2 2 - C/C/H3 - 3   8 - O/C2 - 1 3 - C/C3/OO - 1   9 - CY/C3O - 1 4 - OO/C/H - 1   10 - GAUCHE - 3 5 - C/C2/H2 - 1   11 - DUM1 - 2 6 - C/C4 - 1   12 - DUM2 - 4 Hf S Cp 300 400 500 600 800 1000 1500 -78.37 115.93 49.60 63.52 76.49 87.28 102.86 113.75 .00 CPINF = 150.02 NROTORS: 7 SYMMETRY 27	
C(OOH)ETRAB		3	0	11	2	81	UNITS:KCAL GROUPS 12 Gr # - GROUP ID - Quantity   Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   7 - OO/C/H - 1 2 - C/C4 - 1   8 - CY/C3O - 1 3 - C/C/H2/O - 1   9 - OI - 2 4 - O/C2 - 1   10 - GAUCHE - 3 5 - C/C2/H/O - 1   11 - DUM1 - 2 6 - C/C3/OO - 1   12 - DUM2 - 4 Hf S Cp 300 400 500 600 800 1000 1500 -82.40 114.04 50.29 64.27 77.13 87.77 103.00 113.57 .00 CPINF = 150.02 NROTORS: 7 SYMMETRY 81	
C(OOH)ETRAD		1	0	5	2	27	UNITS:KCAL GROUPS 11 Gr # - GROUP ID - Quantity   Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   7 - C/C2/H2 - 1 2 - C/C4 - 1   8 - CY/C5O - 1 3 - C/C/H2/O - 2   9 - OI - 2 4 - O/C2 - 1   10 - GAUCHE - 1 5 - C/C3/OO - 1   11 - DUM1 - 2 6 - OO/C/H - 1 Hf S Cp 300 400 500 600 800 1000 1500 -100.26 105.93 47.66 62.32 75.95 87.32 103.75 115.17 .00	

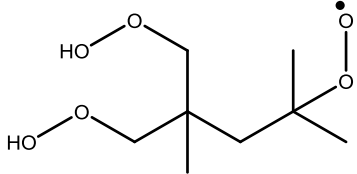
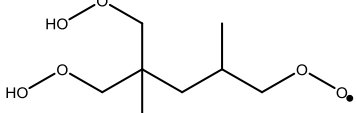
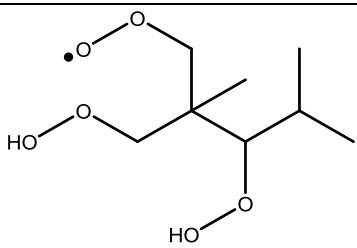
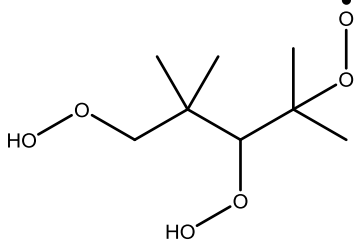
			Gauche	H15	Rotors	OI	Symm.	THERM groups
								CPINF = 152.01 NROTORS: 5 SYMMETRY 27
C(OOH)ETRBD		3	0	7	3	243		UNITS:KCAL GROUPS 12 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   7 - OO/C/H - 1 2 - C/C4 - 1   8 - CY/C3O - 1 3 - C/C2/H/O - 1   9 - OI - 3 4 - O/C2 - 1   10 - GAUCHE - 3 5 - C/C/H2/O - 1   11 - DUM1 - 2 6 - C/C3/OO - 1   12 - DUM2 - 4 Hf S Cp 300 400 500 600 800 1000 1500 -82.40 113.22 50.29 64.27 77.13 87.77 103.00 113.57 .00 CPINF = 150.02 NROTORS: 7 SYMMETRY 243
C(OOH)ETRDD		3	0	7	2	81		UNITS:KCAL GROUPS 13 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   8 - C/C/H2/O - 1 2 - C/C4 - 1   9 - CY/C3O - 1 3 - C/C2/H2 - 1   10 - GAUCHE - 3 4 - C/C3/OO - 1   11 - OI - 2 5 - OO/C/H - 1   12 - DUM1 - 2 6 - C/C/H2/O - 1   13 - DUM2 - 4 7 - O/C2 - 1 Hf S Cp 300 400 500 600 800 1000 1500 -78.37 115.12 49.60 63.52 76.49 87.28 102.86 113.75 .00 CPINF = 150.02 NROTORS: 7 SYMMETRY 81
D(OOH)ETRAA		3	0	7	2	9		UNITS:KCAL GROUPS 12 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 2   7 - C/C/H2/O - 2 2 - C/C3/H - 1   8 - O/C2 - 1 3 - C/C/H2/OO - 1   9 - CY/C3O - 1 4 - OO/C/H - 1   10 - OI - 2 5 - C/C2/H2 - 1   11 - GAUCHE - 3 6 - C/C4 - 1   12 - DUM2 - 4 Hf S Cp 300 400 500 600 800 1000 1500 -72.02 123.05 48.57 62.75 76.03 87.03 102.90 113.92 .00 CPINF = 150.02 NROTORS: 7 SYMMETRY 9
D(OOH)ETRAB		3	0	7	3	27		UNITS:KCAL GROUPS 12 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   7 - C/C/H2/O - 1 2 - C/C3/H - 1   8 - C/C4 - 1 3 - C/C/H2/OO - 1   9 - CY/C3O - 1 4 - OO/C/H - 1   10 - GAUCHE - 3 5 - C/C2/H/O - 1   11 - OI - 3 6 - O/C2 - 1   12 - DUM2 - 4

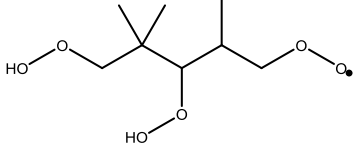
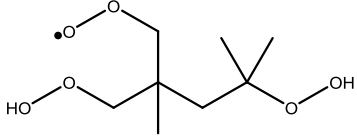
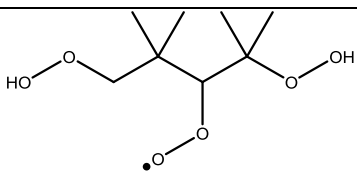
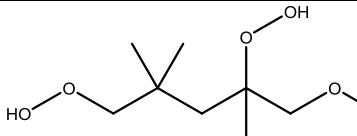
			Gauche	H15	Rotors	OI	Symm.	THERM groups
								Hf S Cp 300 400 500 600 800 1000 1500 -76.05 121.16 49.26 63.50 76.67 87.52 103.04 113.74 .00 CPINF = 150.02 NROTORS: 7 SYMMETRY 27
D(OOH)ETRAC		2	0	6	2	27	UNITS:KCAL GROUPS 11 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   7 - C/C/H2/OO - 1 2 - C/C4 - 1   8 - OO/C/H - 1 3 - C/C/H2/O - 1   9 - CY/C4O - 1 4 - O/C2 - 1   10 - GAUCHE - 2 5 - C/C2/H2 - 1   11 - OI - 2 6 - C/C3/O - 1 Hf S Cp 300 400 500 600 800 1000 1500 -95.35 117.90 47.79 61.85 75.16 86.39 103.07 114.57 .00 CPINF = 151.01 NROTORS: 6 SYMMETRY 27	
D(OOH)ETRAD		1	0	5	2	9	UNITS:KCAL GROUPS 11 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 2   7 - C/C/H2/OO - 1 2 - C/C4 - 1   8 - OO/C/H - 1 3 - C/C/H2/O - 2   9 - GAUCHE - 1 4 - O/C2 - 1   10 - OI - 2 5 - C/C3/H - 1   11 - CY/C5O - 1 6 - C/C2/H2 - 1 Hf S Cp 300 400 500 600 800 1000 1500 -93.91 111.68 46.63 61.55 75.49 87.07 103.79 115.34 .00 CPINF = 152.01 NROTORS: 5 SYMMETRY 9	
D(OOH)ETRBC		3	0	8	3	243	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - CY/C2O - 1 2 - C/C4 - 1   7 - C/C/H2/OO - 1 3 - C/C2/H/O - 1   8 - OO/C/H - 1 4 - O/C2 - 1   9 - OI - 3 5 - C/C3/O - 1   10 - GAUCHE - 3 Hf S Cp 300 400 500 600 800 1000 1500 -76.81 118.38 52.33 65.65 78.07 88.49 103.85 114.45 .00 CPINF = 149.02 NROTORS: 8 SYMMETRY 243	
D(OOH)ETRBD		3	0	7	3	81	UNITS:KCAL GROUPS 12 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   7 - CY/C3O - 1 2 - C/C4 - 1   8 - C/C/H2/OO - 1 3 - C/C2/H/O - 1   9 - OO/C/H - 1 4 - O/C2 - 1   10 - GAUCHE - 3 5 - C/C/H2/O - 1   11 - OI - 3	

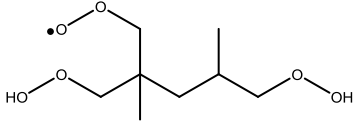
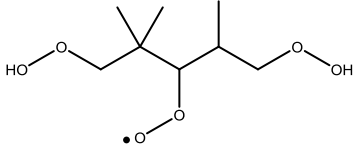
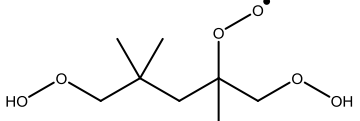
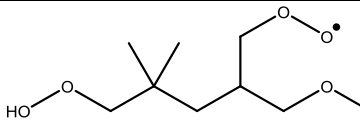


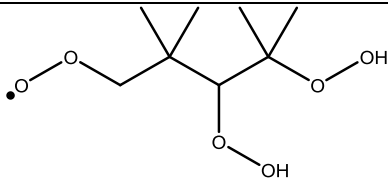
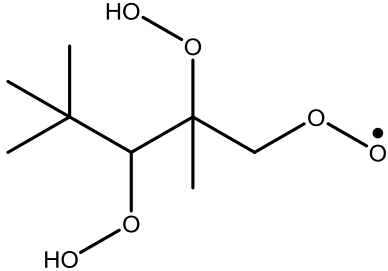
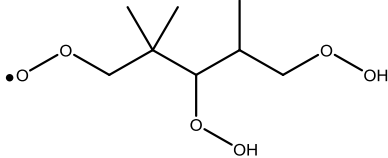
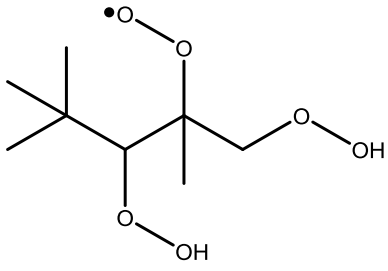
			Gauche	H15	Rotors	OI	Symm.	THERM groups
								6 - C/C3/H - 1   12 - DUM2 - 4 Hf S Cp 300 400 500 600 800 1000 1500 -76.05 118.98 49.26 63.50 76.67 87.52 103.04 113.74 .00 CPINF = 150.02 NROTORS: 7 SYMMETRY 81
	D(OOH)ETRC		3	0	8	2	81	UNITS:KCAL GROUPS 11 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - GAUCHE - 3   7 - O/C2 - 1 2 - OI - 2   8 - C/C/H2/O - 1 3 - C/C/H3 - 3   9 - CY/C2O - 1 4 - C/C4 - 1   10 - C/C/H2/OO - 1 5 - C/C2/H2 - 1   11 - OO/C/H - 1 6 - C/C3/O - 1 Hf S Cp 300 400 500 600 800 1000 1500 -72.78 120.28 51.64 64.90 77.43 88.00 103.71 114.63 .00 CPINF = 149.02 NROTORS: 8 SYMMETRY 81
OHP	XC8OOHA		1	0	8	1	81	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 2   6 - CD/C2 - 1 2 - C/C3/CD - 1   7 - C/CD/H3 - 2 3 - C/C/H2/OO - 1   8 - GAUCHE - 1 4 - OO/C/H - 1   9 - OI - 1 5 - CD/C/H - 1 Hf S Cp 300 400 500 600 800 1000 1500 -46.72 119.90 49.98 62.49 73.57 82.96 96.89 107.05 .00 CPINF = 143.06 NROTORS: 8 SYMMETRY 81
	YC8OOHA		2	0	8	1	27	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 2   6 - CD/C2 - 1 2 - C/C4 - 1   7 - CD/H2 - 1 3 - C/C/H2/OO - 1   8 - C/CD/H3 - 1 4 - OO/C/H - 1   9 - GAUCHE - 2 5 - C/C/CD/H2 - 1   10 - OI - 1 Hf S Cp 300 400 500 600 800 1000 1500 -45.98 120.83 49.57 61.96 73.30 83.24 98.78 109.65 .00 CPINF = 143.06 NROTORS: 8 SYMMETRY 27
	YC8OOHB		2	0	8	2	243	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - CD/H2 - 1 2 - C/C4 - 1   7 - C/CD/H3 - 1 3 - C/C/CD/H/OO - 1   8 - OI - 2 4 - OO/C/H - 1   9 - GAUCHE - 2 5 - CD/C2 - 1 Hf S Cp 300 400 500 600 800 1000 1500 -46.53 115.52 50.62 64.19 75.83 85.94 101.60 111.90 .00

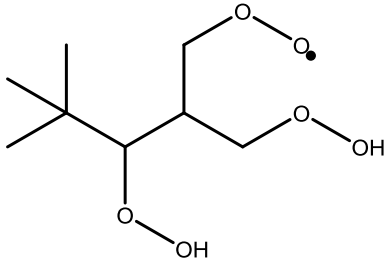
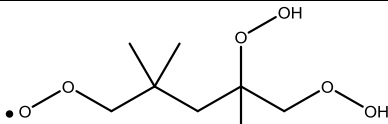
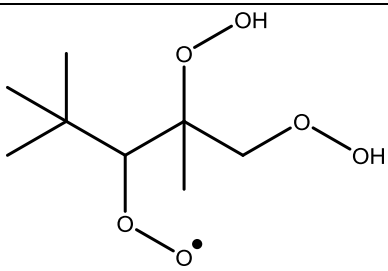
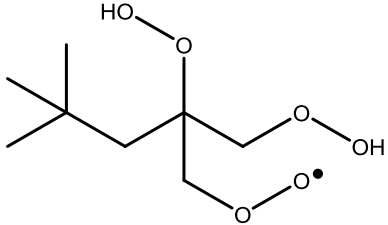
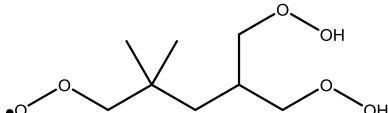
			Gauche	H15	Rotors	OI	Symm.	THERM groups
								CPINF = 143.06 NROTORS: 8 SYMMETRY 243
	XC8OOHD		1	0	8	1	243	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - C/CD/H2/OO - 1 2 - C/C3/CD - 1   7 - OO/C/H - 1 3 - CD/C2 - 1   8 - GAUCHE - 1 4 - CD/C/H - 1   9 - OI - 1 5 - C/CD/H3 - 1 Hf S Cp 300 400 500 600 800 1000 1500 -43.40 120.19 51.23 64.53 75.37 85.01 98.79 108.88 .00 CPINF = 143.06 NROTORS: 8 SYMMETRY 243
	YC8OOHD		2	0	8	1	81	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - C/CD/H2/OO - 1 2 - C/C4 - 1   7 - OO/C/H - 1 3 - C/C/CD/H2 - 1   8 - OI - 1 4 - CD/C2 - 1   9 - GAUCHE - 2 5 - CD/H2 - 1 Hf S Cp 300 400 500 600 800 1000 1500 -42.66 121.13 50.82 64.00 75.10 85.29 100.68 111.48 .00 CPINF = 143.06 NROTORS: 8 SYMMETRY 81
OOP(OOH)2	C8(OOH)AA-AO2		3	0	13	3	9	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - OI - 3   6 - C/C/H2/OO - 3 2 - C/C/H3 - 2   7 - OO/C/H - 3 3 - C/C3/H - 1   8 - GAUCHE - 3 4 - C/C2/H2 - 1   9 - ALPEROX - 1 5 - C/C4 - 1 Hf S Cp 300 400 500 600 800 1000 1500 -77.30 158.80 65.91 80.87 93.98 105.12 122.09 133.78 .00 CPINF = 167.90 NROTORS:13 SYMMETRY 9
	C8(OOH)AA-BO2		3	0	13	4	27	UNITS:KCAL GROUPS 8 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   5 - C/C4 - 1 2 - C/C3/H - 1   6 - C/C/H2/OO - 1 3 - C/C2/H/OO - 2   7 - OI - 4 4 - OO/C/H - 3   8 - GAUCHE - 3 Hf S Cp 300 400 500 600 800 1000 1500 -113.50 134.95 68.87 84.27 97.29 108.51 124.27 135.21 .00 CPINF = 173.86 NROTORS:13 SYMMETRY 27

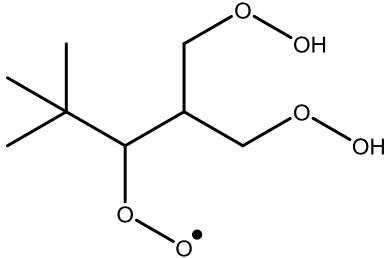
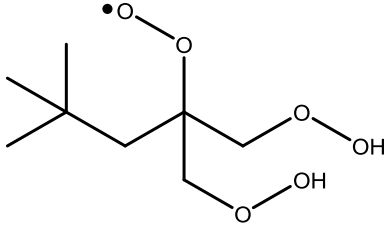
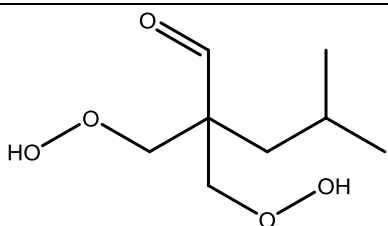
			Gauche	H15	Rotors	OI	Symm.	THERM groups
C8(OOH)AA-CO2		3	0	13	3	27	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - OI - 3 2 - C/C3/OO - 1   7 - C/C/H2/OO - 2 3 - OO/C/H - 3   8 - GAUCHE - 3 4 - C/C2/H2 - 1   9 - ALPEROX - 1 5 - C/C4 - 1 Hf S Cp 300 400 500 600 800 1000 1500 -85.65 153.05 66.94 81.64 94.44 105.37 122.05 133.61 .00 CPINF = 167.90 NROTORS:13 SYMMETRY 27	
C8(OOH)AA-DO2		3	0	13	4	9	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 2   6 - C/C4 - 1 2 - C/C3/H - 1   7 - OI - 4 3 - C/C/H2/OO - 3   8 - GAUCHE - 3 4 - OO/C/H - 3   9 - ALPEROX - 1 5 - C/C2/H2 - 1 Hf S Cp 300 400 500 600 800 1000 1500 -77.30 160.17 65.91 80.87 93.98 105.12 122.09 133.78 .00 CPINF = 167.90 NROTORS:13 SYMMETRY 9	
C8(OOH)AB-AO2		3	0	13	5	27	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - C/C/H2/OO - 1 2 - C/C3/H - 1   7 - OI - 5 3 - C/C2/H/OO - 1   8 - GAUCHE - 3 4 - OO/C/H - 3   9 - ALPEROX - 1 5 - C/C4 - 1 Hf S Cp 300 400 500 600 800 1000 1500 -83.31 181.59 69.49 84.91 97.62 109.16 125.92 137.65 .00 CPINF = 167.90 NROTORS:13 SYMMETRY 27	
C8(OOH)AB-CO2		3	0	13	4	81	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - OI - 4   6 - C/C4 - 1 2 - C/C/H3 - 4   7 - C/C/H2/OO - 1 3 - C/C3/OO - 1   8 - GAUCHE - 3 4 - OO/C/H - 3   9 - ALPEROX - 1 5 - C/C2/H/OO - 1 Hf S Cp 300 400 500 600 800 1000 1500 -89.67 150.80 68.15 82.78 95.36 106.24 122.32 133.54 .00 CPINF = 167.90 NROTORS:13 SYMMETRY 81	

			Gauche	H15	Rotors	OI	Symm.	THERM groups
C8(OOH)AB-DO2		3	0	13	5	27	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - C/C4 - 1 2 - C/C3/H - 1   7 - OI - 5 3 - C/C/H2/OO - 2   8 - GAUCHE - 3 4 - OO/C/H - 3   9 - ALPEROX - 1 5 - C/C2/H/OO - 1 Hf S Cp 300 400 500 600 800 1000 1500 -81.32 157.92 67.12 82.01 94.90 105.99 122.36 133.71 .00 CPINF = 167.90 NROTORS:13 SYMMETRY 27	
C8(OOH)AC-AO2		3	0	13	3	27	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - OI - 3 2 - C/C3/OO - 1   7 - C/C/H2/OO - 2 3 - OO/C/H - 3   8 - GAUCHE - 3 4 - C/C2/H2 - 1   9 - DUM1 - 2 5 - C/C4 - 1   10 - ALPEROX - 1 Hf S Cp 300 400 500 600 800 1000 1500 -83.65 153.05 66.94 81.64 94.44 105.37 122.05 133.61 .00 CPINF = 167.90 NROTORS:13 SYMMETRY 27	
C8(OOH)AC-BO2		3	0	13	4	81	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - OI - 4   6 - C/C4 - 1 2 - C/C/H3 - 4   7 - C/C/H2/OO - 1 3 - C/C3/OO - 1   8 - GAUCHE - 3 4 - OO/C/H - 3   9 - DUM1 - 2 5 - C/C2/H/OO - 1   10 - ALPEROX - 1 Hf S Cp 300 400 500 600 800 1000 1500 -87.67 150.80 68.15 82.78 95.36 106.24 122.32 133.54 .00 CPINF = 167.90 NROTORS:13 SYMMETRY 81	
C8(OOH)AC-DO2		3	0	13	4	27	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - OI - 4   6 - C/C2/H2 - 1 2 - C/C/H3 - 3   7 - C/C4 - 1 3 - C/C3/OO - 1   8 - GAUCHE - 3 4 - OO/C/H - 3   9 - DUM1 - 2 5 - C/C/H2/OO - 2   10 - ALPEROX - 1 Hf S Cp 300 400 500 600 800 1000 1500 -83.65 154.42 66.94 81.64 94.44 105.37 122.05 133.61 .00 CPINF = 167.90 NROTORS:13 SYMMETRY 27	

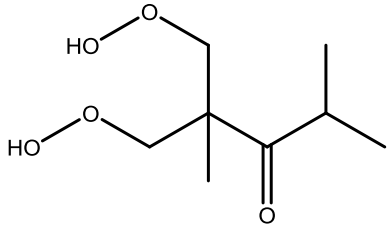
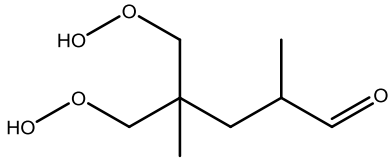
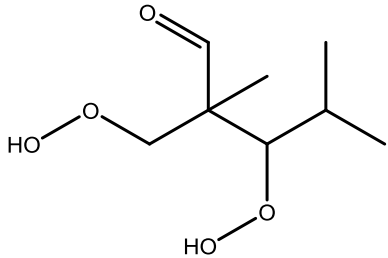
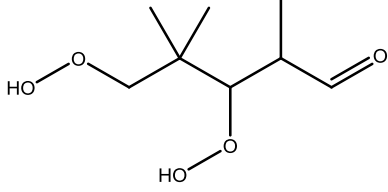
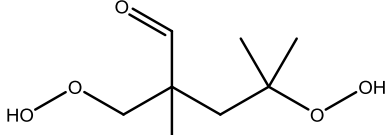
			Gauche	H15	Rotors	OI	Symm.	THERM groups
C8(OOH)AD-AO2		3	0	13	5	9	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 2   6 - C/C4 - 1 2 - C/C3/H - 1   7 - OI - 5 3 - C/C/H2/OO - 3   8 - GAUCHE - 3 4 - OO/C/H - 3   9 - ALPEROX - 1 5 - C/C2/H2 - 1 Hf S Cp 300 400 500 600 800 1000 1500 -77.30 161.54 65.91 80.87 93.98 105.12 122.09 133.78 .00 CPINF = 167.90 NROTORS:13 SYMMETRY 9	
C8(OOH)AD-BO2		3	0	13	5	27	UNITS:KCAL GROUPS 8 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   5 - C/C2/H/OO - 1 2 - C/C3/H - 1   6 - C/C4 - 1 3 - C/C/H2/OO - 2   7 - OI - 5 4 - OO/C/H - 3   8 - GAUCHE - 3 Hf S Cp 300 400 500 600 800 1000 1500 -114.49 158.40 68.29 83.79 97.18 108.73 125.61 137.39 .00 CPINF = 173.86 NROTORS:13 SYMMETRY 27 CREATION DATE: 4/19/16 ENDSPECIES	
C8(OOH)AD-CO2		3	0	13	4	27	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - OI - 4   6 - C/C2/H2 - 1 2 - C/C/H3 - 3   7 - C/C4 - 1 3 - C/C3/OO - 1   8 - GAUCHE - 3 4 - OO/C/H - 3   9 - ALPEROX - 1 5 - C/C/H2/OO - 2 Hf S Cp 300 400 500 600 800 1000 1500 -85.65 154.42 66.94 81.64 94.44 105.37 122.05 133.61 .00 CPINF = 167.90 NROTORS:13 SYMMETRY 27	
C8(OOH)AD-DO2		3	0	13	4	9	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 2   6 - C/C2/H2 - 1 2 - OI - 4   7 - C/C4 - 1 3 - C/C3/H - 1   8 - GAUCHE - 3 4 - C/C/H2/OO - 3   9 - ALPEROX - 1 5 - OO/C/H - 3 Hf S Cp 300 400 500 600 800 1000 1500 -77.30 160.17 65.91 80.87 93.98 105.12 122.09 133.78 .00 CPINF = 167.90 NROTORS:13 SYMMETRY 9	

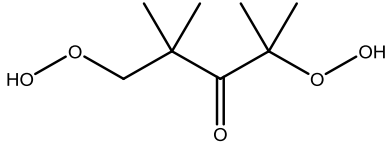
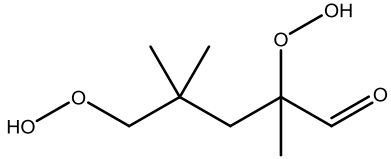
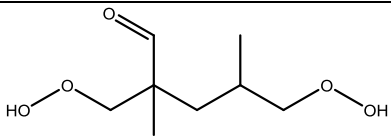
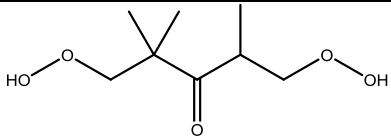
			Gauche	H15	Rotors	OI	Symm.	THERM groups
C8(OOH)BC-AO2		3	0	13	4	81	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - OI - 4   6 - C/C4 - 1 2 - C/C/H3 - 4   7 - C/C/H2/OO - 1 3 - C/C3/OO - 1   8 - GAUCHE - 3 4 - OO/C/H - 3   9 - DUM1 - 2 5 - C/C2/H/OO - 1   10 - ALPEROX - 1 Hf S Cp 300 400 500 600 800 1000 1500 -87.67 150.80 68.15 82.78 95.36 106.24 122.32 133.54 .00 CPINF = 167.90 NROTORS:13 SYMMETRY 81	
C8(OOH)BC-DO2		3	0	13	5	243	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - C/C4 - 1 2 - C/C3/OO - 1   7 - OI - 5 3 - OO/C/H - 3   8 - GAUCHE - 3 4 - C/C/H2/OO - 1   9 - DUM1 - 2 5 - C/C2/H/OO - 1   10 - ALPEROX - 1 Hf S Cp 300 400 500 600 800 1000 1500 -87.67 149.99 68.15 82.78 95.36 106.24 122.32 133.54 .00 CPINF = 167.90 NROTORS:13 SYMMETRY 243	
C8(OOH)BD-AO2		3	0	13	5	27	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - C/C4 - 1 2 - C/C3/H - 1   7 - OI - 5 3 - C/C/H2/OO - 2   8 - GAUCHE - 3 4 - OO/C/H - 3   9 - ALPEROX - 1 5 - C/C2/H/OO - 1 Hf S Cp 300 400 500 600 800 1000 1500 -81.32 157.92 67.12 82.01 94.90 105.99 122.36 133.71 .00 CPINF = 167.90 NROTORS:13 SYMMETRY 27	
C8(OOH)BD-CO2		3	0	13	5	243	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - C/C4 - 1 2 - C/C3/OO - 1   7 - OI - 5 3 - OO/C/H - 3   8 - GAUCHE - 3 4 - C/C/H2/OO - 1   9 - ALPEROX - 1 5 - C/C2/H/OO - 1 Hf S Cp 300 400 500 600 800 1000 1500 -89.67 149.99 68.15 82.78 95.36 106.24 122.32 133.54 .00 CPINF = 167.90 NROTORS:13 SYMMETRY 243	

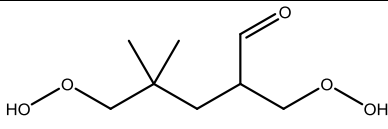
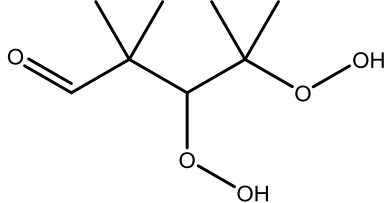
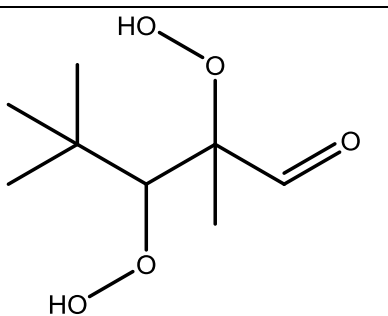
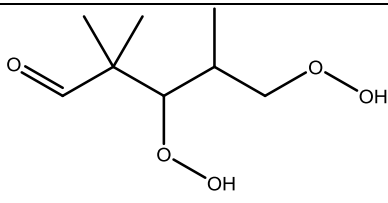
			Gauche	H15	Rotors	OI	Symm.	THERM groups
C8(OOH)BD-DO2		3	0	13	5	81	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - C/C/H2/OO - 2 2 - C/C4 - 1   7 - OI - 5 3 - C/C2/H/OO - 1   8 - GAUCHE - 3 4 - OO/C/H - 3   9 - ALPEROX - 1 5 - C/C3/H - 1 Hf S Cp 300 400 500 600 800 1000 1500 -81.32 155.74 67.12 82.01 94.90 105.99 122.36 133.71 .00 CPINF = 167.90 NROTORS:13 SYMMETRY 81	
C8(OOH)CD-AO2		3	0	13	4	27	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - OI - 4   6 - C/C2/H2 - 1 2 - C/C/H3 - 3   7 - C/C4 - 1 3 - C/C3/OO - 1   8 - GAUCHE - 3 4 - OO/C/H - 3   9 - DUM1 - 2 5 - C/C/H2/OO - 2   10 - ALPEROX - 1 Hf S Cp 300 400 500 600 800 1000 1500 -83.65 154.42 66.94 81.64 94.44 105.37 122.05 133.61 .00 CPINF = 167.90 NROTORS:13 SYMMETRY 27	
C8(OOH)CD-BO2		3	0	13	5	243	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   6 - C/C4 - 1 2 - C/C3/OO - 1   7 - OI - 5 3 - OO/C/H - 3   8 - GAUCHE - 3 4 - C/C/H2/OO - 1   9 - DUM1 - 2 5 - C/C2/H/OO - 1   10 - ALPEROX - 1 Hf S Cp 300 400 500 600 800 1000 1500 -87.67 149.99 68.15 82.78 95.36 106.24 122.32 133.54 .00 CPINF = 167.90 NROTORS:13 SYMMETRY 243	
C8(OOH)CD-DO2		3	0	13	2	81	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - C/C/H2/OO - 2 2 - C/C4 - 1   7 - OI - 3 3 - C/C2/H2 - 1   8 - GAUCHE - 3 4 - C/C3/OO - 1   9 - DUM1 - 2 5 - OO/C/H - 3   10 - ALPEROX - 1 Hf S Cp 300 400 500 600 800 1000 1500 -83.65 150.87 66.94 81.64 94.44 105.37 122.05 133.61 .00 CPINF = 167.90 NROTORS:13 SYMMETRY 81	
C8(OOH)DD-AO2		3	0	13		9	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity	

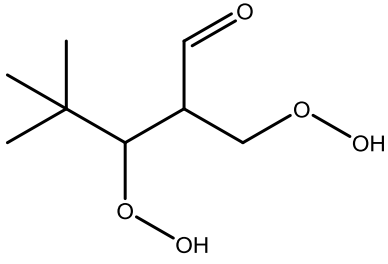
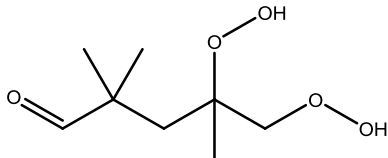
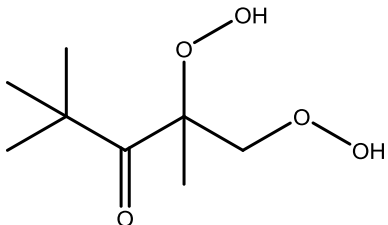
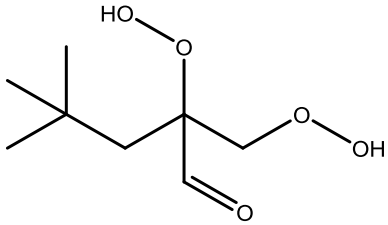
			Gauche	H15	Rotors	OI	Symm.	THERM groups
								1 - C/C/H3 - 2   6 - C/C2/H2 - 1 2 - OI - 3   7 - C/C4 - 1 3 - C/C3/H - 1   8 - GAUCHE - 3 4 - C/C/H2/OO - 3   9 - ALPEROX - 1 5 - OO/C/H - 3 Hf S Cp 300 400 500 600 800 1000 1500 -77.30 158.80 65.91 80.87 93.98 105.12 122.09 133.78 .00 CPINF = 167.90 NROTORS:13 SYMMETRY 9
	C8(OOH)DD-BO2		3	0	13	4	81	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - C/C/H2/OO - 2 2 - C/C4 - 1   7 - OI - 4 3 - C/C2/H/OO - 1   8 - GAUCHE - 3 4 - OO/C/H - 3   9 - ALPEROX - 1 5 - C/C3/H - 1 Hf S Cp 300 400 500 600 800 1000 1500 -81.32 154.37 67.12 82.01 94.90 105.99 122.36 133.71 .00 CPINF = 167.90 NROTORS:13 SYMMETRY 81
	C8(OOH)DD-CO2		3	0	13	3	81	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - C/C/H2/OO - 2 2 - C/C4 - 1   7 - OI - 3 3 - C/C2/H2 - 1   8 - GAUCHE - 3 4 - C/C3/OO - 1   9 - ALPEROX - 1 5 - OO/C/H - 3 Hf S Cp 300 400 500 600 800 1000 1500 -85.65 150.87 66.94 81.64 94.44 105.37 122.05 133.61 .00 CPINF = 167.90 NROTORS:13 SYMMETRY 81
KDHP	C8(OOH)AA-KETA		3	0	11	2	9	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 2   6 - C/C3/CO - 1 2 - C/C3/H - 1   7 - CO/C/H - 1 3 - C/C2/H2 - 1   8 - OI - 2 4 - C/C/H2/OO - 2   9 - GAUCHE - 3 5 - OO/C/H - 2 Hf S Cp 300 400 500 600 800 1000 1500 -112.77 148.76 60.23 73.98 85.86 95.86 110.31 121.01 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 9

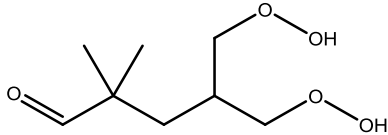
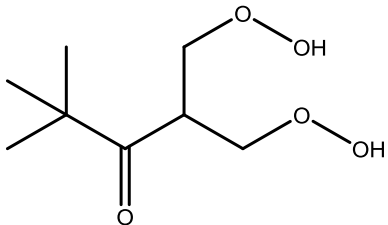


			Gauche	H15	Rotors	OI	Symm.	THERM groups
C8(OOH)AA-KETB		3	0	11	2	27	UNITS:KCAL GROUPS 8 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   5 - OO/C/H - 2 2 - CO/C2 - 1   6 - C/C/H2/OO - 2 3 - C/C2/CO/H - 1   7 - OI - 2 4 - C/C3/CO - 1   8 - GAUCHE - 3 Hf S Cp 300 400 500 600 800 1000 1500 -120.58 147.85 59.79 72.40 83.83 93.65 108.02 118.69 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 27	
C8(OOH)AA-KETD		3	0	11	3	9	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 2   6 - C/C2/CO/H - 1 2 - C/C/H2/OO - 2   7 - CO/C/H - 1 3 - OO/C/H - 2   8 - OI - 3 4 - C/C4 - 1   9 - GAUCHE - 3 5 - C/C2/H2 - 1 Hf S Cp 300 400 500 600 800 1000 1500 -111.83 148.41 60.49 73.85 86.07 96.90 113.12 124.45 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 9	
C8(OOH)AB-KETA		3	0	11	4	27	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - CO/C/H - 1 2 - C/C3/H - 1   7 - C/C3/CO - 1 3 - C/C2/H/OO - 1   8 - OI - 4 4 - OO/C/H - 2   9 - GAUCHE - 3 5 - C/C/H2/OO - 1 Hf S Cp 300 400 500 600 800 1000 1500 -116.79 147.88 61.44 75.12 86.78 96.73 110.58 120.94 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 27	
C8(OOH)AB-KETD		3	0	11	4	27	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - OO/C/H - 2 2 - C/C2/CO/H - 1   7 - OI - 4 3 - CO/C/H - 1   8 - C/C4 - 1 4 - C/C2/H/OO - 1   9 - GAUCHE - 3 5 - C/C/H2/OO - 1 Hf S Cp 300 400 500 600 800 1000 1500 -115.85 146.16 61.70 74.99 86.99 97.77 113.39 124.38 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 27	
C8(OOH)AC-KETA		3	0	11	3	27	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - C/C/H2/OO - 1 2 - C/C3/OO - 1   7 - CO/C/H - 1	

			Gauche	H15	Rotors	OI	Symm.	THERM groups
								3 - OO/C/H - 2   8 - GAUCHE - 3 4 - C/C2/H2 - 1   9 - OI - 3 5 - C/C3/CO - 1   10 - DUM1 - 2 Hf S Cp 300 400 500 600 800 1000 1500 -119.12 144.38 61.26 74.75 86.32 96.11 110.27 120.84 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 27
C8(OOH)AC-KETB		3	0	11	2	81	UNITS:KCAL GROUPS 11 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   7 - O/H/O - 1 2 - C/C3/CO - 1   8 - OO/C/H - 1 3 - C/C/H2/OO - 1   9 - OI - 2 4 - CO/C2 - 1   10 - GAUCHE - 3 5 - C/C2/CO/O - 1   11 - DUM1 - 2 6 - O/C/O - 1 Hf S Cp 300 400 500 600 800 1000 1500 -122.64 143.89 60.75 74.14 86.04 96.20 110.84 121.62 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 81	
C8(OOH)AC-KETD		3	0	11	3	27	UNITS:KCAL GROUPS 12 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   7 - C/C2/H2 - 1 2 - C/C2/CO/O - 1   8 - C/C4 - 1 3 - O/C/O - 1   9 - C/C/H2/OO - 1 4 - O/H/O - 1   10 - OI - 3 5 - CO/C/H - 1   11 - GAUCHE - 3 6 - OO/C/H - 1   12 - DUM1 - 2 Hf S Cp 300 400 500 600 800 1000 1500 -113.89 144.45 61.45 75.59 88.28 99.45 115.94 127.38 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 27	
C8(OOH)AD-KETA		3	0	11	4	9	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 2   6 - C/C3/CO - 1 2 - C/C3/H - 1   7 - CO/C/H - 1 3 - C/C/H2/OO - 2   8 - OI - 4 4 - OO/C/H - 2   9 - GAUCHE - 3 5 - C/C2/H2 - 1 Hf S Cp 300 400 500 600 800 1000 1500 -112.77 151.50 60.23 73.98 85.86 95.86 110.31 121.01 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 9	
C8(OOH)AD-KETB		3	0	11	3	27	UNITS:KCAL GROUPS 8 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   5 - CO/C2 - 1 2 - C/C2/CO/H - 1   6 - C/C3/CO - 1 3 - C/C/H2/OO - 2   7 - OI - 3 4 - OO/C/H - 2   8 - GAUCHE - 3	

			Gauche	H15	Rotors	OI	Symm.	THERM groups
								Hf S Cp 300 400 500 600 800 1000 1500 -120.58 149.22 59.79 72.40 83.83 93.65 108.02 118.69 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 27
C8(OOH)AD-KETD		3	0	11	3	9	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 2   6 - C/C2/CO/H - 1 2 - C/C4 - 1   7 - CO/C/H - 1 3 - C/C/H2/OO - 2   8 - OI - 3 4 - OO/C/H - 2   9 - GAUCHE - 3 5 - C/C2/H2 - 1 Hf S Cp 300 400 500 600 800 1000 1500 -111.83 148.41 60.49 73.85 86.07 96.90 113.12 124.45 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 9	
C8(OOH)BC-KETA		3	0	11	3	81	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - GAUCHE - 3   6 - C/C2/H/OO - 1 2 - OI - 3   7 - C/C3/CO - 1 3 - C/C/H3 - 4   8 - CO/C/H - 1 4 - C/C3/OO - 1   9 - DUM1 - 2 5 - OO/C/H - 2 Hf S Cp 300 400 500 600 800 1000 1500 -123.14 140.76 62.47 75.89 87.24 96.98 110.54 120.77 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 81	
C8(OOH)BC-KETD		3	0	11	4	243	UNITS:KCAL GROUPS 11 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 4   7 - O/H/O - 1 2 - C/C4 - 1   8 - CO/C/H - 1 3 - C/C2/H/OO - 1   9 - OI - 4 4 - OO/C/H - 1   10 - GAUCHE - 3 5 - C/C2/CO/O - 1   11 - DUM1 - 2 6 - O/C/O - 1 Hf S Cp 300 400 500 600 800 1000 1500 -117.91 140.01 62.66 76.73 89.20 100.32 116.21 127.31 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 243	
C8(OOH)BD-KETA		3	0	11	4	27	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - C/C3/CO - 1 2 - C/C/H2/OO - 1   7 - CO/C/H - 1 3 - OO/C/H - 2   8 - OI - 4 4 - C/C3/H - 1   9 - GAUCHE - 3 5 - C/C2/H/OO - 1 Hf S Cp 300 400 500 600 800 1000 1500 -116.79 147.88 61.44 75.12 86.78 96.73 110.58 120.94 .00 CPINF = 157.97	

		Gauche	H15	Rotors	OI	Symm.	THERM groups
							NROTORS:11 SYMMETRY 27
C8(OOH)BD-KETD		3	0	11	4	81	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - C/C2/CO/H - 1 2 - C/C4 - 1   7 - CO/C/H - 1 3 - OI - 4   8 - C/C/H2/OO - 1 4 - C/C2/H/OO - 1   9 - GAUCHE - 3 5 - OO/C/H - 2 Hf S Cp 300 400 500 600 800 1000 1500 -115.85 143.98 61.70 74.99 86.99 97.77 113.39 124.38 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 81
C8(OOH)CD-KETA		3	0	11	3	27	UNITS:KCAL GROUPS 10 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   6 - CO/C/H - 1 2 - C/C3/OO - 1   7 - OI - 3 3 - OO/C/H - 2   8 - C/C/H2/OO - 1 4 - C/C2/H2 - 1   9 - GAUCHE - 3 5 - C/C3/CO - 1   10 - DUM1 - 2 Hf S Cp 300 400 500 600 800 1000 1500 -119.12 144.38 61.26 74.75 86.32 96.11 110.27 120.84 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 27
C8(OOH)CD-KETB		3	0	11	3	243	UNITS:KCAL GROUPS 11 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - OI - 3   7 - C/C/H2/OO - 1 2 - C/C/H3 - 4   8 - CO/C2 - 1 3 - C/C2/CO/O - 1   9 - C/C3/CO - 1 4 - O/C/O - 1   10 - GAUCHE - 3 5 - O/H/O - 1   11 - DUM1 - 2 6 - OO/C/H - 1 Hf S Cp 300 400 500 600 800 1000 1500 -122.64 143.07 60.75 74.14 86.04 96.20 110.84 121.62 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 243
C8(OOH)CD-KETD		3	0	11	3	81	UNITS:KCAL GROUPS 12 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 3   7 - OO/C/H - 2 2 - C/C4 - 1   8 - C/C/H2/OO - 1 3 - C/C2/H2 - 1   9 - CO/C/H - 1 4 - C/C2/CO/O - 1   10 - OI - 3 5 - O/C/O - 1   11 - GAUCHE - 3 6 - O/H/O - 1   12 - DUM1 - 2 Hf S Cp 300 400 500 600 800 1000 1500 -134.49 180.91 70.97 86.64 99.84 111.98 129.34 141.43 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 81

			Gauche	H15	Rotors	OI	Symm.	THERM groups
	C8(OOH)DD-KETA		3	0	11	2	9	UNITS:KCAL GROUPS 9 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H3 - 2   6 - C/C3/CO - 1 2 - C/C/H2/OO - 2   7 - CO/C/H - 1 3 - OO/C/H - 2   8 - OI - 2 4 - C/C3/H - 1   9 - GAUCHE - 3 5 - C/C2/H2 - 1 Hf S Cp 300 400 500 600 800 1000 1500 -112.77 148.76 60.23 73.98 85.86 95.86 110.31 121.01 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 9
	C8(OOH)DD-KETB		3	0	11	2	81	UNITS:KCAL GROUPS 8 Gr # - GROUP ID - Quantity Gr # - GROUP ID - Quantity 1 - C/C/H2/OO - 2   5 - C/C4 - 1 2 - OO/C/H - 2   6 - C/C/H3 - 3 3 - C/C2/CO/H - 1   7 - OI - 2 4 - CO/C2 - 1   8 - GAUCHE - 3 Hf S Cp 300 400 500 600 800 1000 1500 -119.00 144.01 59.99 72.89 84.92 95.57 111.82 123.07 .00 CPINF = 157.97 NROTORS:11 SYMMETRY 81