

Supplement3_thermdat

THERMO

	300.000	1000.000	5000.000									
cyC6H12				C	6H	12O	0	OG	200.000	6000.00	1000.0	1
	1.32145970E+01	3.58243434E-02	-1.32110852E-05						2.17202521E-09	-1.31730622E-13		2
	-2.28092102E+04	-5.53518322E+01	4.04357527E+00						-6.19608335E-03	1.76622274E-04		3
	-2.22968474E-07	8.63668578E-11	-1.69203544E+04						8.52527441E+00	-1.48294969E+04		4
cyC6H11				C	6H	11O	0	OG	200.000	6000.00	1000.0	1
	0.57261502E+01	0.49173558E-01	-0.23796767E-04						0.54208507E-08	-0.47445368E-12		2
	0.10056946E+04	-0.11973133E+02	-0.10741222E+01						0.34294293E-01	0.64592225E-04		3
	-0.10261825E-06	0.40853054E-10	0.45268762E+04						0.31367410E+02	0.61161896E+04		4
cyC6H10				C	6H	10O	0	OG	200.000	6000.00	1000.0	1
	0.39442769E+01	0.47473657E-01	-0.23199637E-04						0.53766657E-08	-0.47931014E-12		2
	-0.44509693E+04	-0.29390438E+00	-0.27517028E+01						0.48912768E-01	0.19511676E-04		3
	-0.59644226E-07	0.27082294E-10	-0.19687471E+04						0.37948748E+02	-0.54967525E+03		4
cyC6H9		A05/05C		6H	9O	0	OG		200.000	6000.00	1000.0	1
	0.48230902E+01	0.43906891E-01	-0.21524326E-04						0.49885999E-08	-0.44431982E-12		2
	0.10570260E+05	-0.50750458E+01	-0.43595073E+01						0.60597409E-01	-0.13999007E-04		3
	-0.24483785E-07	0.13990165E-10	0.13380358E+05						0.44118420E+02	0.14606688E+05		4
cyC6H8_13		T 1/90C		6H	8O	0	OG		200.000	6000.00	1000	1
	0.57911078E+01	0.38887445E-01	-0.19353118E-04						0.45417154E-08	-0.40833894E-12		2
	0.85461589E+04	-0.95072842E+01	0.17881209E+01						0.14442450E-01	0.95904952E-04		3
	-0.14190881E-06	0.59226641E-10	0.11037921E+05						0.18868425E+02	0.12806110E+05		4
cyC6H8_14		T 1/90C		6H	8O	0	OG		200.000	6000.00	1000	1
	0.60072048E+01	0.38131392E-01	-0.18750123E-04						0.43570611E-08	-0.38863868E-12		2
	0.88163073E+04	-0.18395532E+02	0.19112107E+01						0.14754449E-01	0.91475839E-04		3
	-0.13476207E-06	0.55972633E-10	0.11366314E+05						0.10445281E+02	0.13158528E+05		4
cyC6H110				C	6H	11O	1	OG	300.000	5000.00	1000.0	1
	0.32637255E+01	0.58784029E-01	-0.29394748E-04						0.68775840E-08	-0.61578610E-12		2
	-0.12963675E+05	0.23642621E+01	-0.38078981E+01						0.57665454E-01	0.17189370E-04		3
	-0.53677606E-07	0.21536939E-10	-0.10152550E+05						0.43686705E+02	-0.86709165E+04		4
cyC6H1000H				C	6H	11O	2	G	300.00	5000.00	1000.0	1
	0.92613052E+01	0.55409862E-01	-0.27657605E-04						0.64468604E-08	-0.57481577E-12		2
	-0.11509255E+05	-0.23691117E+02	-0.38172431E+01						0.81355661E-01	-0.31709899E-04		3
	-0.10022352E-07	0.70721153E-11	-0.74649250E+04						0.46310647E+02	-0.52862641E+04		4
a-cyC6H1000H				C	6H	11O	2	G	300.00	5000.00	1000.0	1
	0.91017065E+01	0.52091518E-01	-0.25944131E-04						0.60871367E-08	-0.54676862E-12		2
	-0.89772135E+04	-0.22534805E+02	-0.17750211E+01						0.71010961E-01	-0.22421128E-04		3
	-0.11354775E-07	0.53233922E-11	-0.55480956E+04						0.36264454E+02	-0.31416887E+04		4
cyOOC6H1000H				C	6H	11O	4	G	300.000	5000.00	1000.0	1
	0.20094503E+01	0.74073855E-01	-0.39254193E-04						0.96576588E-08	-0.90066937E-12		2
	-0.25674718E+05	0.20565845E+02	-0.17398958E+01						0.71686526E-01	0.72801188E-05		3
	-0.58960561E-07	0.27307535E-10	-0.24730231E+05						0.41406273E+02	-0.22104883E+05		4
cyOONC6H900H				C	6H	11O	4	G	300.000	5000.00	1376.0	1
	0.13296721E+02	0.56179584E-01	-0.28298589E-04						0.66759657E-08	-0.60158400E-12		2
	-0.21992272E+05	-0.40186252E+02	-0.55936490E+01						0.12238953E+00	-0.13187643E-03		3
	0.97940639E-07	-0.35615990E-10	-0.17494214E+05						0.54214822E+02	-0.14713736E+05		4
cyC6H1100				C	6H	11O	2	G	300.00	5000.00	1000.0	1
	-0.20839567E+00	0.68532755E-01	-0.35407414E-04						0.85310323E-08	-0.78298305E-12		2
	-0.13493035E+05	0.24862162E+02	0.76560000E+00						0.29242014E-01	0.99097744E-04		3
	-0.14795512E-06	0.59505351E-10	-0.12592840E+05						0.27262169E+02	-0.10455858E+05		4
cyC6H100b				C	6H	10O	1	OG	300.000	5000.000	1000.000	1
	-0.94946020E+01	0.80553090E-01	-0.44208480E-04						0.11132126E-07	-0.10563421E-11		2
	-0.15606945E+05	0.65125482E+02	0.29262009E+01						0.65415817E-02	0.15371109E-03		3
	-0.21344824E-06	0.87175623E-10	-0.18496486E+05						0.71794684E+01	-0.16357950E+05		4

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cyC6H100c	C	6H	100	1	OG	300.000	5000.000	1000.000	1
-0.95853077E+01	0.80577563E-01	-0.44174188E-04	0.11116295E-07	-0.10544255E-11					2
-0.25530791E+05	0.61862506E+02	0.16169856E+01	0.11188534E-01	0.14771115E-03					3
-0.21071414E-06	0.87058128E-10	-0.28165251E+05	0.98415047E+01	-0.26258119E+05					4
cyC6H100d	C	6H	100	1	OG	300.000	5000.000	1000.000	1
-0.66687497E+00	0.60687596E-01	-0.30099302E-04	0.70125266E-08	-0.62731530E-12					2
-0.31167893E+05	0.26362479E+02	-0.78489570E+01	0.93504999E-01	-0.94472350E-04					3
0.71093411E-07	-0.25979669E-10	-0.29886581E+05	0.60321458E+02	-0.28779168E+05					4
cyC6H100a	C	6H	100	1	OG	300.00	5000.000	1000.0	1
-0.80846809E+01	0.78416058E-01	-0.42966125E-04	0.10802297E-07	-0.10236452E-11					2
-0.15124674E+05	0.60499401E+02	-0.16543292E+01	0.42696025E-01	0.62179263E-04					3
-0.11687253E-06	0.50777343E-10	-0.17184963E+05	0.28835473E+02	-0.15440221E+05					4
cyOC6H90OH	C	6H	100	3	OG	300.00	5000.000	1000.0	1
0.31662570E+00	0.69003372E-01	-0.36037339E-04	0.87559801E-08	-0.80895897E-12					2
-0.42944421E+05	0.28684832E+02	-0.83287424E+01	0.12266269E+00	-0.15487972E-03					3
0.12834888E-06	-0.46584898E-10	-0.42257621E+05	0.65746476E+02	-0.40428193E+05					4
cyC6H90	C	6H	90	1	OG	300.000	5000.000	1369.000	1
-0.74704407E+01	0.74757622E-01	-0.41387678E-04	0.10473466E-07	-0.99677029E-12					2
0.60398853E+04	0.59505359E+02	-0.23187144E+01	0.50151874E-01	0.34652255E-04					3
-0.86353641E-07	0.39225621E-10	0.40066875E+04	0.32724381E+02	0.56964157E+04					4
cyC6H900	C	6H	90	2	OG	300.000	5000.000	1000.000	1
-0.15752926E+01	0.63566897E-01	-0.33475432E-04	0.82122290E-08	-0.76530877E-12					2
0.22864969E+04	0.36636285E+02	-0.16012226E+01	0.51507380E-01	0.25977280E-04					3
-0.73889337E-07	0.33956656E-10	0.21056130E+04	0.37835261E+02	0.40149146E+04					4
cyC6H80OH	C	6H	90	2	G	300.00	5000.00	1000.0	1
0.65407841E+01	0.49378665E-01	-0.25554660E-04	0.62086740E-08	-0.57419865E-12					2
0.87506338E+04	-0.54098324E+01	0.47690303E+00	0.60864654E-01	-0.18222490E-04					3
-0.15492520E-07	0.83620658E-11	0.10265509E+05	0.26325566E+02	0.12922781E+05					4