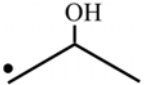
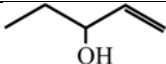
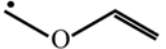
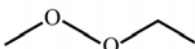
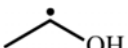
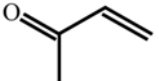



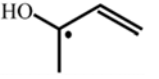



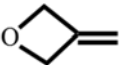

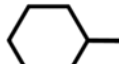

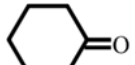
Table S1. Comparison of thermodynamic values between calculated and available literature data for selective validation species which containing certain number of new Benson groups.

New Group	Formula	Molecule	Ref	$\Delta H_f^0 /$ kJ·mol ⁻¹	$S^0 /$ J·mol ⁻¹ ·K ⁻¹	$C_p(T) / \text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$						
						300	400	500	600	800	1000	1500
<i>G1</i>	C ₃ H ₇ O		p.w. [*] , [1]	-61.71	320.43	93.30	112.57	129.23	143.49	165.00	179.34	205.61
			[2]	-64.92	319.52	96.89	115.41	131.13	144.29	165.07	180.99	206.78
			[3] ^a	-61.56	326.06	94.21	112.85	128.48	141.87	163.18	179.66	204.97
			[3] ^b	-64.79	318.39	95.64	113.99	129.75	142.87	163.56	179.41	205.36
			[4]	-96.14	-	-	-	-	-	-	-	-
			[5]	-61.446	325.62	94.89	112.86	128.33	141.70	162.60	178.90	205.24
MAD^c				12.48	3.20	1.22	1.06	1.01	0.98	0.99	0.71	0.63
<i>G2</i>	C ₅ H ₁₀ O		p.w.	-184.19	372.37	121.62	154.53	183.75	208.87	250.98	268.23	304.96
			[3] ^d	-191.46	385.24	125.46	157.15	183.76	206.56	242.79	269.24	301.77
DF^e				7.27	12.87	3.84	2.62	0.01	2.31	8.19	1.01	3.19
<i>G4</i>	C ₃ H ₅ O		p.w.	90.21	303.07	79.07	92.10	103.94	114.62	135.19	145.65	166.68
			[3]	96.36	305.36	79.28	97.02	110.75	122.07	140.26	153.09	171.13
DF^e				6.15	2.29	0.21	4.91	6.81	7.45	5.06	7.44	4.45
<i>G4, G16</i>	C ₃ H ₇ O ₂		p.w.	36.10	358.33	103.37	125.64	144.53	161.08	188.09	205.90	241.85
			[2]	31.39	359.94	110.60	130.46	148.01	162.81	186.05	203.32	229.98
			[3]	28.38	341.46	107.47	130.71	150.15	166.32	192.36	213.10	239.68
MAD				3.18	8.36	2.96	2.33	2.31	2.18	2.63	4.14	5.16
<i>G6</i>	C ₂ H ₄ OH		p.w., [1]	-55.53	285.13	63.67	76.80	88.93	99.80	116.42	125.12	144.89
			[3]	-55.52	284.79	64.87	77.70	89.26	99.51	115.71	126.93	145.93
			[3] ^f	-54.04	288.94	64.02	76.59	88.14	98.26	113.65	125.60	144.44
			[2]	-58.65	285.08	65.33	78.25	90.12	100.28	116.20	128.16	147.09
			[4]	-60.61	-	-	-	-	-	-	-	-
			[5]	-54.34	284.66	66.04	78.58	89.87	99.48	115.37	127.07	145.88
			[6]	-53.17	-	-	-	-	-	-	-	-
			[7]	-63.95	-	-	-	-	-	-	-	-
			[8]	-55.18	-	-	-	-	-	-	-	-
			[9]	-51.41	280.48	-	-	-	-	-	-	-
[10]	-53.92	288.44	-	-	-	-	-	-	-			
MAD				3.47	2.66	0.86	0.78	0.70	0.67	0.98	1.09	0.92

<i>G7</i>	C ₄ H ₆ O		p.w., [1]	-127.02	321.00	87.56	109.43	129.19	146.05	170.16	187.94	212.38
			[2]	-109.93	322.82	90.37	111.27	130.04	145.88	170.38	187.97	214.35
			[3] ^f	-109.47	327.80	87.49	106.17	124.19	139.86	165.19	184.21	209.29
			[11]	-115.00	320.34	-	-	-	-	-	-	-
			MAD	7.07	2.92	1.34	2.11	2.58	2.88	2.39	1.77	2.08
<i>G8, G15</i>	CH ₂ CHO		p.w., [1]	25.20	268.13	54.96	63.37	70.96	77.80	89.13	97.68	111.28
			[2]	14.00	260.75	54.97	65.12	74.07	81.55	93.26	101.91	114.99
			[3] ^a	18.52	258.53	53.17	63.87	73.11	80.76	92.92	101.11	114.32
			[3] ^f	12.74	264.16	54.32	64.83	73.88	81.38	91.94	99.71	111.26
			[5]	18.39	258.74	53.09	63.95	73.15	80.67	92.38	101.16	114.53
			[9]	10.45	267.52	-	-	-	-	-	-	-
			[12]	15.50	-	-	-	-	-	-	-	-
			[13]	40.45	-	-	-	-	-	-	-	-
MAD	4.83	4.23	0.92	0.64	1.14	1.42	1.64	1.64	1.46			
<i>G9</i>	C ₄ H ₇		p.w., [14]	204.74	317.28	84.76	104.57	122.90	138.97	167.01	181.87	209.29
			[20], [21]	217.20	324.10	84.40	104.40	122.30	137.50	161.50	179.60	210.80
			[3] ^b	208.12	315.46	86.69	105.92	123.31	138.15	161.81	179.70	208.12
			[3] ^f	204.36	321.94	82.76	103.37	121.76	137.44	162.56	180.70	209.38
			[3] ^g	203.20	320.17	88.21	109.31	126.96	141.91	165.22	182.66	210.25
			[5]	208.16	315.59	86.53	105.75	123.31	138.36	161.77	179.74	208.16
			[9]	214.43	316.01	-	-	-	-	-	-	-
			[10]	204.40	316.84	-	-	-	-	-	-	-
MAD	4.82	3.04	1.78	1.89	1.67	1.52	2.07	1.18	0.99			
<i>G10</i>	C ₅ H ₇		p.w., [14]	205.43	323.13	93.88	119.48	141.87	160.83	188.63	209.45	239.67
			[20], [21]	209.00	308.10	95.40	121.10	143.10	161.10	188.00	208.00	240.42
			[3] ^g	205.47	323.01	94.05	120.61	142.63	161.20	189.94	215.21	239.00
			[3] ^f	206.27	317.69	86.74	115.41	138.56	157.58	186.19	207.08	237.67
			MAD	1.46	6.25	3.39	2.24	1.78	1.51	1.35	3.15	1.13
<i>G12</i>	C ₄ H ₇ O		p.w., [1]	-44.08	333.01	97.89	120.74	141.00	158.51	184.59	201.21	229.83
			[2]	-59.73	333.56	111.02	133.22	151.48	166.45	189.52	206.78	234.25
DF			15.65	0.56	13.13	12.48	10.48	7.94	4.93	5.57	4.41	

*: predicted values *a*: RMG. DFT-QCI-thermo *b*: RMG.CBS-QB3-1dHR *c*: Mean Absolute Deviation *d*: RMG. Group Additivity
e: difference with literature data *f*: RMG. Curran-pentane species *g*: RMG. USC-Mech2

Table S2. Comparison of thermodynamic values between calculated and available literature data for selective species, containing ring-correction groups.

Group	Formula	Molecule	Ref	ΔH_f^0 / kJ·mol ⁻¹	S^0 / J·mol ⁻¹ ·K ⁻¹	$C_p(T)$ /J·mol ⁻¹ ·K ⁻¹						
						300	400	500	600	800	1000	1500
RC1	C ₃ H ₆ O	 Methyl oxirane	p.w.*	-91.07	285.11	71.97	93.94	112.90	128.80	151.87	169.77	202.69
			[3] ^a , [14]	-92.77	281.43	72.64	92.56	110.78	126.57	149.77	167.09	192.27
			[3] ^b	-88.46	272.74	78.64	97.51	114.48	129.64	154.14	176.62	210.62
			[5]	-93.21	286.33	72.73	92.38	109.93	124.98	148.39	165.53	191.86
			[11]	-94.68	287.40	72.92	92.99	110.99	126.16	149.68	166.85	193.06
MAD^c				2.13	5.33	2.45	1.90	1.65	1.73	2.02	3.97	7.43
RC2	C ₄ H ₆ O	 Oxetane, 3-methylene	p.w.	18.56	290.90	74.57	100.35	123.44	142.91	170.06	191.04	226.41
			[3] ^a	4.26	290.80	77.68	102.28	122.82	140.29	167.67	187.36	216.58
			[3] ^b	23.91	301.90	75.91	99.79	121.88	141.26	169.87	188.55	219.67
MAD			8.30	5.21	1.27	1.07	0.64	1.08	1.09	1.54	4.10	
RC2	C ₃ H ₆ O	 oxetane	p.w., [14]	-81.11	274.97	61.82	82.56	102.91	120.90	146.60	166.68	203.57
			[3] ^a	-81.09	274.62	61.79	82.56	102.91	120.90	146.60	165.70	193.07
			[3] ^d	-75.05	265.60	61.37	83.10	102.85	120.44	148.21	167.86	200.57
			[11]	-80.54	-	61.94	83.97	104.24	121.31	147.44	166.12	193.93
			[5]	-79.42	274.21	63.54	85.27	105.34	122.47	148.39	166.78	194.79
			[3] ^b	-82.81	272.49	70.60	88.28	107.68	124.69	149.69	168.45	212.51
			[15]	-105.34	270.78	61.95	84.73	105.34	122.35	147.89	165.99	193.28
MAD			8.56	3.01	3.74	2.18	1.88	1.57	1.12	1.04	7.75	
RC6	cyC ₇ H ₁₄	 Methyl-cyclohexane	p.w.	-154.83	334.56	126.98	177.53	223.29	263.28	323.83	366.65	427.42
			[3] ^b	-153.42	340.49	134.52	183.95	229.45	269.78	331.03	370.01	430.51
			[11]	-154.80	343.30	136.70	186.0	229.90	266.80	323.50	364.10	424.50
			[16]	-143.0	-	-	-	-	-	-	-	-
MAD			4.95	3.64	4.16	3.61	3.01	2.66	3.47	2.42	2.45	
RC7	cyC ₆ H ₁₀	 Cyclohexene	p.w., [11]	-4.37	310.31	102.16	139.77	173.10	201.59	244.61	275.32	321.55
			[14]	-4.61	310.56	101.40	138.69	172.75	202.12	244.76	276.05	320.30
			[16]	7.20	-	-	-	-	-	-	-	-
MAD			5.56	-	-	-	-	-	-	-	-	
DF^e				0.04	0.94	0.04	1.08	0.34	0.53	0.16	0.73	1.25
RC6	cyC ₆ H ₁₀ O	 d-cyC ₆ H ₁₀ O	p.w.	-239.27	331.32	111.48	152.36	187.40	218.16	268.12	301.86	358.53
			[3] ^b	-231.67	340.55	122.39	160.54	194.89	224.86	270.01	299.79	340.39
			[3] ^d	-225.68	334.52	120.55	159.81	195.22	226.07	271.84	299.98	352.91
			[11]	-231.1	335.53	121.89	161.88	196.39	225.24	269.47	301.06	-

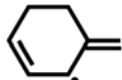


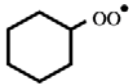
MAD				4.84	3.32	4.44	3.71	3.55	3.16	1.33	0.84	7.58
<i>RC7</i>	cyC ₇ H ₉		p.w.	186.38	326.71	110.44	152.65	188.52	217.93	259.05	290.77	334.01
			[3] ^f	196.47	338.17	113.90	152.72	186.63	214.86	254.01	281.44	324.51
		Methylene cyclohexenyl										
DF				10.09	11.46	3.47	0.07	1.89	3.07	5.04	9.33	9.49
<i>RC8</i>	cyC ₆ H ₈		p.w., [14]	106.47	303.32	94.12	127.57	157.54	182.93	218.85	244.92	281.34
			[3] ^b	104.59	296.65	93.49	127.17	157.26	182.56	217.73	243.12	281.52
			[3] ^g	106.20	303.19	93.60	126.75	157.18	183.48	220.63	242.76	286.92
		1,3-Cyclohexadiene	[11]	104.58	-	94.8	128.55	157.99	182.24	218.7	244.45	282.52
			[16]	120.2	-	-	-	-	-	-	-	-
MAD				5.95	3.11	0.53	0.58	0.30	0.28	0.50	0.76	0.52
*: present work <i>a</i> : RMG, Curran-pentane species <i>b</i> : RMG, Group Additivity <i>c</i> : Mean Absolute Deviation <i>d</i> : RMG, CHO <i>e</i> : Difference with literature data <i>f</i> : RMG, vinylCPD_H <i>g</i> : RMG, CH												

Table A.1. Benson's groups, symmetry numbers and NASA-coefficients for selected species.

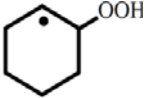
Structure	groups	No.
	C-(C) ₂ (H) ₂	3
	C-(C•)(C)(H) ₂	2
	C•-(C) ₂ (H)	1
	RC10	6

NASA Coefficients					
Species	a ₁	a ₂	a ₃	a ₄	a ₅
cyC ₆ H ₁₁	0.57261502E+01	0.49173558E-01	-0.23796767E-04	0.54208507E-08	-0.47445368E-12
linearity	a ₆	a ₇	a ₈	a ₉	a ₁₀
non-linear	0.10056946E+04	-0.11973133E+02	-0.10741222E+01	0.34294293E-01	0.64592225E-04
Sym. numbers*	a ₁₃	a ₁₂	a ₁₃	a ₁₄	a ₁₅
(2/1)	-0.10261825E-06	0.40853054E-10	0.45268762E+04	0.31367410E+02	0.61161896E+04


*(external/ internal)

Structure	groups	No.
	O-(C)(O•)	1
	C-(C) ₂ (H) ₂	5
	C-(C) ₂ (O)(H)	1
	RC10	6

NASA Coefficients					
Species	a ₁	a ₂	a ₃	a ₄	a ₅
cyC ₆ H ₁₁ OO•	-0.20839567E+00	0.68532755E-01	-0.35407414E-04	0.85310323E-08	-0.78298305E-12
linearity	a ₆	a ₇	a ₈	a ₉	a ₁₀
non-linear	-0.13493035E+05	0.24862162E+02	0.76560000E+00	0.29242014E-01	0.99097744E-04
Sym. numbers	a ₁₃	a ₁₂	a ₁₃	a ₁₄	a ₁₅
(2/1)	-0.14795512E-06	0.59505351E-10	-0.12592840E+05	0.27262169E+02	-0.10455858E+05

Structure	groups	No.
	O-(O)(C)	1
	O-(O)(H)	1
	C-(C) ₂ (H) ₂	3
	C-(C•)(C)(H) ₂	1
	C-(C•)(C)(O)(H)	1
	C•-(C) ₂ (H)	1
	RC10	6

NASA Coefficients					
Species	a ₁	a ₂	a ₃	a ₄	a ₅
a-cyC ₆ H ₁₀ OOH	0.91017065E+01	0.52091518E-01	-0.25944131E-04	0.60871367E-08	-0.54676862E-12
linearity	a ₆	a ₇	a ₈	a ₉	a ₁₀
non-linear	-0.89772135E+04	-0.22534805E+02	-0.17750211E+01	0.71010961E-01	-0.22421128E-04
Sym. numbers	a ₁₃	a ₁₂	a ₁₃	a ₁₄	a ₁₅
(1/1)	-0.11354775E-07	0.53233922E-11	-0.55480956E+04	0.36264454E+02	-0.31416887E+04

Structure	groups	No.
	O-(C) ₂	1
	C-(C) ₂ (O)(H)	2
	C-(C) ₂ (H) ₂	4
	RC10	4
	RC1	1

NASA Coefficients					
Species	a ₁	a ₂	a ₃	a ₄	a ₅
a-cyC ₆ H ₁₀ O	-0.80846809E+01	0.78416058E-01	-0.42966125E-04	0.10802297E-07	-0.10236452E-11
linearity	a ₆	a ₇	a ₈	a ₉	a ₁₀
non-linear	-0.15124674E+05	0.60499401E+02	-0.16543292E+01	0.42696025E-01	0.62179263E-04
Sym. numbers	a ₁₃	a ₁₂	a ₁₃	a ₁₄	a ₁₅
(2/1)	-0.11687253E-06	0.50777343E-10	-0.17184963E+05	0.28835473E+02	-0.15440221E+05

Structure	groups	No.
	O-(C) ₂	1
	C-(C) ₂ (O)(H)	2
	C-(C) ₂ (H) ₂	4
	RC10	3
	RC2	1

NASA Coefficients

Species	a ₁	a ₂	a ₃	a ₄	a ₅
b-cyC ₆ H ₁₀ O	-0.94946020E+01	0.80553090E-01	-0.44208480E-04	0.11132126E-07	-0.10563421E-11
linearity	a ₆	a ₇	a ₈	a ₉	a ₁₀
non-linear	-0.15606945E+05	0.65125482E+02	0.29262009E+01	0.65415817E-02	0.15371109E-03
Sym. numbers	a ₁₃	a ₁₂	a ₁₃	a ₁₄	a ₁₅
(2/1)	-0.21344824E-06	0.87175623E-10	-0.18496486E+05	0.71794684E+01	-0.16357950E+05

Structure	groups	No.
	O-(C) ₂	1
	C-(C) ₂ (O)(H)	2
	C-(C) ₂ (H) ₂	4
	RC10	2
	RC3	1

NASA Coefficients

Species	a ₁	a ₂	a ₃	a ₄	a ₅
c-cyC ₆ H ₁₀ O	-0.95853077E+01	0.80577563E-01	-0.44174188E-04	0.11116295E-07	-0.10544255E-11
linearity	a ₆	a ₇	a ₈	a ₉	a ₁₀
non-linear	-0.25530791E+05	0.61862506E+02	0.16169856E+01	0.11188534E-01	0.14771115E-03
Sym. numbers	a ₁₃	a ₁₂	a ₁₃	a ₁₄	a ₁₅
(4/1)	-0.21071414E-06	0.87058128E-10	-0.28165251E+05	0.98415047E+01	-0.26258119E+05

Structure	groups	No.
	CO-(C) ₂	1
	C-(CO)(C)(H) ₂	2
	C-(C) ₂ (H) ₂	3
	RC10	6

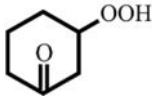
NASA Coefficients

Species	a ₁	a ₂	a ₃	a ₄	a ₅
d-cyC ₆ H ₁₀ O	-0.66687497E+00	0.60687596E-01	-0.30099302E-04	0.70125266E-08	-0.62731530E-12
linearity	a ₆	a ₇	a ₈	a ₉	a ₁₀
non-linear	-0.31167893E+05	0.26362479E+02	-0.78489570E+01	0.93504999E-01	-0.94472350E-04
Sym. numbers	a ₁₃	a ₁₂	a ₁₃	a ₁₄	a ₁₅
(2/1)	0.71093411E-07	-0.25979669E-10	-0.29886581E+05	0.60321458E+02	-0.28779168E+05

Structure	groups	No.
	O-(C)(O•)	1
	O-(O)(C)	1
	O-(O)(H)	1
	C-(C) ₂ (O)(H)	2
	C-(C) ₂ (H) ₂	4
	RC10	6


NASA Coefficients

Species	a ₁	a ₂	a ₃	a ₄	a ₅
cy-OOC ₆ H ₁₀ OOH	0.20094503E+01	0.74073855E-01	-0.39254193E-04	0.96576588E-08	-0.90066937E-12
linearity	a ₆	a ₇	a ₈	a ₉	a ₁₀
non-linear	-0.25674718E+05	0.20565845E+02	-0.17398958E+01	0.71686526E-01	0.72801188E-05
Sym. numbers	a ₁₃	a ₁₂	a ₁₃	a ₁₄	a ₁₅
(1/1)	-0.58960561E-07	0.27307535E-10	-0.24730231E+05	0.41406273E+02	-0.22104883E+05

Structure	groups	No.
	O-(O)(C)	1
	O-(O)(H)	1
	C-(C)2(O)(H)	1
	C-(C)2(H)2	2
	C-(CO)(C)(H)2	2
	CO-(C)2	1
	RC10	6

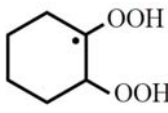
NASA Coefficients

Species	a ₁	a ₂	a ₃	a ₄	a ₅
cyOC ₆ H ₉ OOH	0.31662570E+00	0.69003372E-01	-0.36037339E-04	0.87559801E-08	-0.80895897E-12
linearity	a ₆	a ₇	a ₈	a ₉	a ₁₀
non-linear	-0.42944421E+05	0.28684832E+02	-0.83287424E+01	0.12266269E+00	-0.15487972E-03
Sym. numbers	a ₁₃	a ₁₂	a ₁₃	a ₁₄	a ₁₅
(1/1)	0.12834888E-06	-0.46584898E-10	-0.42257621E+05	0.65746476E+02	-0.40428193E+05

Structure	groups	No.
	C _d -(C)(H)	2
	C-(C _d)(C)(H)2	2
	C-(C)2(H)2	2
	RC9	1

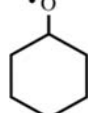
NASA Coefficients

Species	a ₁	a ₂	a ₃	a ₄	a ₅
cyC ₆ H ₁₀	0.39442769E+01	0.47473657E-01	-0.23199637E-04	0.53766657E-08	-0.47931014E-12
linearity	a ₆	a ₇	a ₈	a ₉	a ₁₀
non-linear	-0.44509693E+04	-0.29390438E+00	-0.27517028E+01	0.48912768E-01	0.19511676E-04
Sym. numbers	a ₁₃	a ₁₂	a ₁₃	a ₁₄	a ₁₅
(2/1)	-0.59644226E-07	0.27082294E-10	-0.19687471E+04	0.37948748E+02	-0.54967525E+03

Structure	groups	No.
	O-(O)(C)	1
	O-(C•)(O)	1
	O-(O)(H)	2
	C•-(C)2(O)	1
	C-(C•)(C)(H)2	1
	C-(C)2(H)2	3
	C-(C•)(C)(O)(H)	1
	RC10	6

NASA Coefficients

Species	a ₁	a ₂	a ₃	a ₄	a ₅
cyC ₆ H ₉ (OOH) ₂	0.13296721E+02	0.56179584E-01	-0.28298589E-04	0.66759657E-08	-0.60158400E-12
linearity	a ₆	a ₇	a ₈	a ₉	a ₁₀
non-linear	-0.21992272E+05	-0.40186252E+02	-0.55936490E+01	0.12238953E+00	-0.13187643E-03
Sym. numbers	a ₁₃	a ₁₂	a ₁₃	a ₁₄	a ₁₅
(1/1)	0.97940639E-07	-0.35615990E-10	-0.17494214E+05	0.54214822E+02	-0.14713736E+05

Structure	groups	No.
	C-(O•)(C)2(H)	1
	C-(C)2(H)2	5
	RC10	6


NASA Coefficients

Species	a ₁	a ₂	a ₃	a ₄	a ₅
cyC ₆ H ₁₁ O	0.32637255E+01	0.58784029E-01	-0.29394748E-04	0.68775840E-08	-0.61578610E-12
linearity	a ₆	a ₇	a ₈	a ₉	a ₁₀
non-linear	-0.12963675E+05	0.23642621E+01	-0.38078981E+01	0.57665454E-01	0.17189370E-04
Sym. numbers	a ₁₃	a ₁₂	a ₁₃	a ₁₄	a ₁₅
(2/1)	-0.53677606E-07	0.21536939E-10	-0.10152550E+05	0.43686705E+02	-0.86709165E+04

Structure	groups	No.
	C-(C) ₂ (O)(H)	2
	C•-(C) ₂ (H)	1
	C-(C•)(C)(H) ₂	2
	C-(C) ₂ (H) ₂	1
	O-(C) ₂	1
	RC1, RC10	1, 4


NASA Coefficients

Species	a ₁	a ₂	a ₃	a ₄	a ₅
a-cyC ₆ H ₉ O	-0.74704407E+01	0.74757622E-01	-0.41387678E-04	0.10473466E-07	-0.99677029E-12
linearity	a ₆	a ₇	a ₈	a ₉	a ₁₀
non-linear	0.60398853E+04	0.59505359E+02	-0.23187144E+01	0.50151874E-01	0.34652255E-04
Sym. numbers	a ₁₃	a ₁₂	a ₁₃	a ₁₄	a ₁₅
(1/1)	-0.86353641E-07	0.39225621E-10	0.40066875E+04	0.32724381E+02	0.56964157E+04

Structure	groups	No.
	C•-(H)(C)(C _d)	1
	C _d -(C•)(H)	1
	C _d -(C)(H)	1
	C-(C _d)(C)(H) ₂	1
	C-(C•)(C)(H) ₂	1
	C-(C) ₂ (H) ₂	1
	RC7	1


NASA Coefficients

Species	a ₁	a ₂	a ₃	a ₄	a ₅
1,3-cyC ₆ H ₉	0.48230902E+01	0.43906891E-01	-0.21524326E-04	0.49885999E-08	-0.44431982E-12
linearity	a ₆	a ₇	a ₈	a ₉	a ₁₀
non-linear	0.10570260E+05	-0.50750458E+01	-0.43595073E+01	0.60597409E-01	-0.13999007E-04
Sym. numbers	a ₁₃	a ₁₂	a ₁₃	a ₁₄	a ₁₅
(1/1)	-0.24483785E-07	0.13990165E-10	0.13380358E+05	0.44118420E+02	0.14606688E+05

Structure	groups	No.
	C•-(C) ₂ (H)	1
	C-(C•)(C)(H) ₂	1
	C _d -(C)(H)	2
	C-(C _d)(C)(H) ₂	1
	C-(C•)(C _d)(H) ₂	1
	RC7	1


NASA Coefficients

Species	a ₁	a ₂	a ₃	a ₄	a ₅
1,4-cyC ₆ H ₉	0.39653625E+01	0.44688860E-01	-0.22101693E-04	0.51691476E-08	-0.46400342E-12
linearity	a ₆	a ₇	a ₈	a ₉	a ₁₀
non-linear	0.18469954E+05	0.15519697E+01	0.11513849E+01	0.24349750E-01	0.68252173E-04
Sym. numbers	a ₁₃	a ₁₂	a ₁₃	a ₁₄	a ₁₅
(1/1)	-0.10615713E-06	0.43656116E-10	0.20343077E+05	0.22231144E+02	0.22180659E+05

Structure	groups	No.
	C _d -(C)(H)	4
	C-(C _d) ₂ (H) ₂	2
	RC9	1

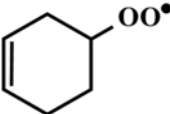
NASA Coefficients

Species	a ₁	a ₂	a ₃	a ₄	a ₅
1,4-cyC ₆ H ₈	0.60072048E+01	0.38131392E-01	-0.18750123E-04	0.43570611E-08	-0.38863868E-12
linearity	a ₆	a ₇	a ₈	a ₉	a ₁₀
non-linear	0.88163073E+04	-0.18395532E+02	0.19112107E+01	0.14754449E-01	0.91475839E-04
Sym. numbers	a ₁₃	a ₁₂	a ₁₃	a ₁₄	a ₁₅
(3/1)	-0.13476207E-06	0.55972633E-10	0.11366314E+05	0.10445281E+02	0.13158528E+05

Structure	groups	No.
	C _d -(C)(H)	2
	C-(C _d)(C)(H) ₂	2
	C _d -(C _d)(H)	2
	RC8	1

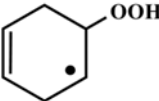
NASA Coefficients

Species	a ₁	a ₂	a ₃	a ₄	a ₅
1,3-cyC ₆ H ₈	0.57911078E+01	0.38887445E-01	-0.19353118E-04	0.45417154E-08	-0.40833894E-12
linearity	a₆	a₇	a₈	a₉	a₁₀
non-linear	0.85461589E+04	-0.95072842E+01	0.17881209E+01	0.14442450E-01	0.95904952E-04
Sym. numbers	a₁₃	a₁₂	a₁₃	a₁₄	a₁₅
(2/1)	-0.14190881E-06	0.59226641E-10	0.11037921E+05	0.18868425E+02	0.12806110E+05

Structure	groups	No.
	O-(C)(O•)	1
	C _d -(C)(H)	2
	C-(C _d)(C)(H) ₂	2
	C-(C) ₂ (H) ₂	1
	C-(C) ₂ (O)(H)	1
	RC7	1

NASA Coefficients

Species	a ₁	a ₂	a ₃	a ₄	a ₅
cyC ₆ H ₉ OO	-0.15752926E+01	0.63566897E-01	-0.33475432E-04	0.82122290E-08	-0.76530877E-12
linearity	a₆	a₇	a₈	a₉	a₁₀
non-linear	0.22864969E+04	0.36636285E+02	-0.16012226E+01	0.51507380E-01	0.25977280E-04
Sym. numbers	a₁₃	a₁₂	a₁₃	a₁₄	a₁₅
(1/1)	-0.73889337E-07	0.33956656E-10	0.21056130E+04	0.37835261E+02	0.40149146E+04

Structure	groups	No.
	O-(O)(C)	1
	O-(O)(H)	1
	C _d -(C)(H)	2
	C-(C _d)(C)(H) ₂	1
	C-(C•)(C _d)(H) ₂	1
	C-(C•)(C)(O)(H)	1
	C•-(C) ₂ (H)	1
	RC7	1

NASA Coefficients

Species	a ₁	a ₂	a ₃	a ₄	a ₅
cyC ₆ H ₈ OOH	0.65407841E+01	0.49378665E-01	-0.25554660E-04	0.62086740E-08	-0.57419865E-12
linearity	a₆	a₇	a₈	a₉	a₁₀
non-linear	0.87506338E+04	-0.54098324E+01	0.47690303E+00	0.60864654E-01	-0.18222490E-04
Sym. numbers	a₁₃	a₁₂	a₁₃	a₁₄	a₁₅
(1/1)	-0.15492520E-07	0.83620658E-11	0.10265509E+05	0.26325566E+02	0.12922781E+05

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List of tables

Table S1. Comparison of thermodynamic values between calculated and available literature data for selective validation species which containing certain number of new Benson groups.

Table S2. Comparison of thermodynamic values between calculated and available literature data for selective species, containing ring-correction groups.

Table A.1. Benson's groups, symmetry numbers and NASA-coefficients for selected species.