Thermodynamics of Chlorinated Phenols, Polychlorinated Dibenzo-*p*-Dioxins, Polychlorinated Dibenzofurans, Derived Radicals, and Intermediate Species

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The thermodynamics of 31 chlorinated phenols, polychlorinated dibenzo-*p*-dioxins, polychlorinated dibenzofurans, and some chlorinated cyclo–C_5 compounds have been calculated. Twelve of these species are radicals. Additionally the thermodynamic properties of temperature dependent tables ($T=0$ K–6000 K) of the ideal gas phase thermodynamic properties are listed, together with recommended values for the structure, vibrational frequencies, and enthalpy of formation either found in the literature or calculated. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1521164]

Key words: chlorinated and polychlorinated cyclo–C_5 compounds; dibenzo-*p*-dioxins and dibenzo-furans; Gaussian 98 and MOPAC calculations; phenols; thermodynamics.

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1. Introduction

It has been over 20 years since it was first proposed that the major sources of poly-chlorinated dibenzo-*p*-dioxins and polychlorinated dibenzofurans (PCDD/F or ''dioxins'' for short) and many other chlorinated hydrocarbons are combustion and thermal processes.[1–7] Formation of PCDD/F and related compounds in combustion systems have been attributed to so-called *de novo* synthesis from particulate carbon[8–12] and formation from chlorinated aromatic precursors such as 2,4,6-trichlorophenol.[13–17]

Both gas-phase and surface-mediated formation pathways may exist.[17–19] Publication of a gas-phase kinetic model for the formation of PCDD from chlorinated phenols, which suggested that gas-phase pathways were too slow to be important sources of PCDD/F, resulted in greater attention to the surface-mediated pathways from researchers active in the field (Shaub and Tsang[20]). However, more recent studies of gas-phase formation suggest that PCDD/F can be rapidly formed via several different gas-phase pathways involving phenoxy radicals.[17,21–23]

Although the original kinetic model has been re-evaluated several times in the literature, no substantive improvements have been attempted.[17,24,25] Neither newly proposed pathways nor thermochemistry were incorporated into the models.

In this paper, we report the calculations of the thermodynamic properties of 31 chlorinated molecules and radicals that we have incorporated into an expanded model of purely gas phase PCDD formation from chlorinated phenols (Khachatryan *et al.*[53]) that incorporates the results of more recent experimental and mechanistic studies.[20–22] (See Table 2.) The species, names, and chemical formulas are listed below. The structure of each model is given in Fig. 1.

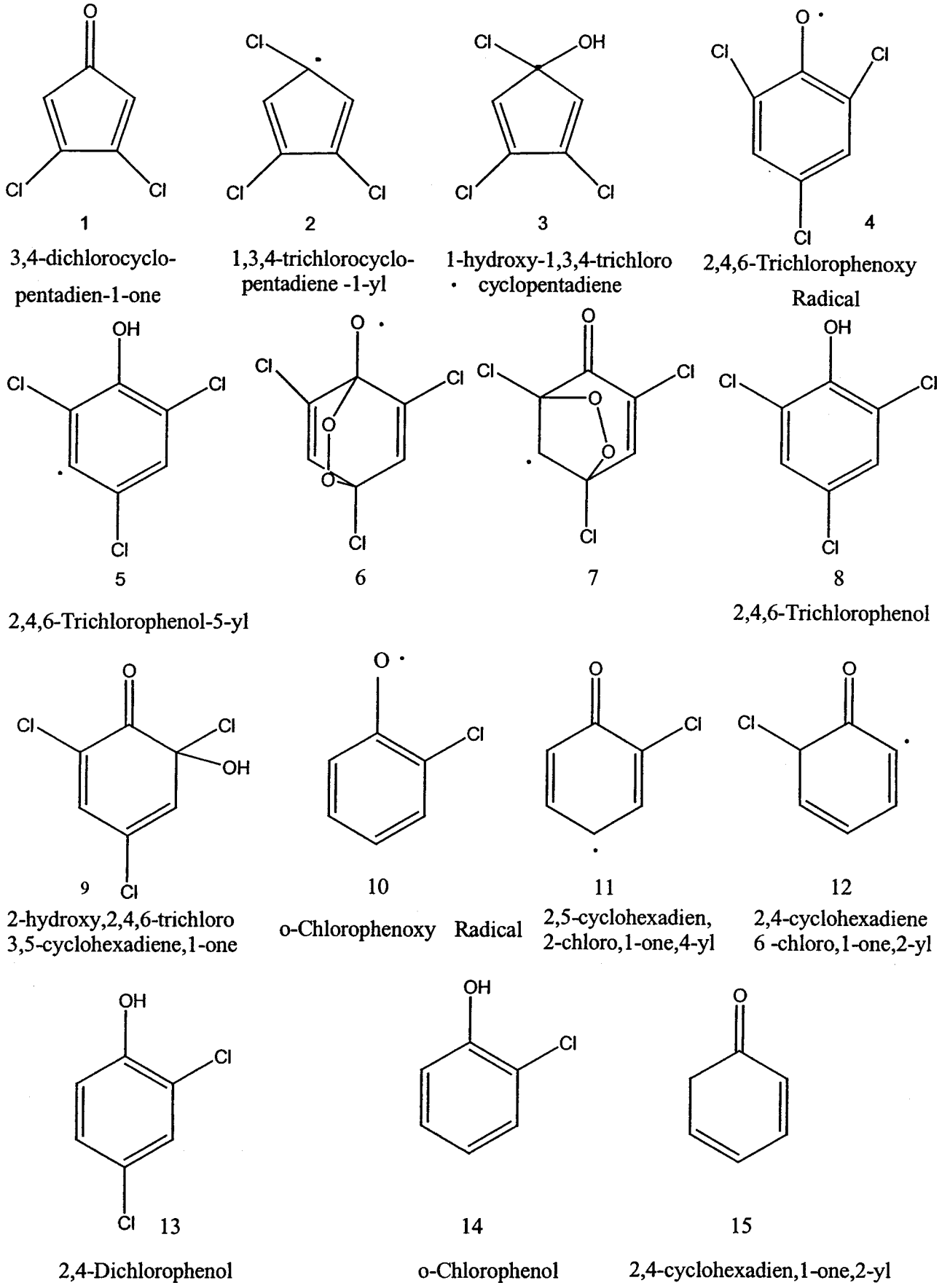
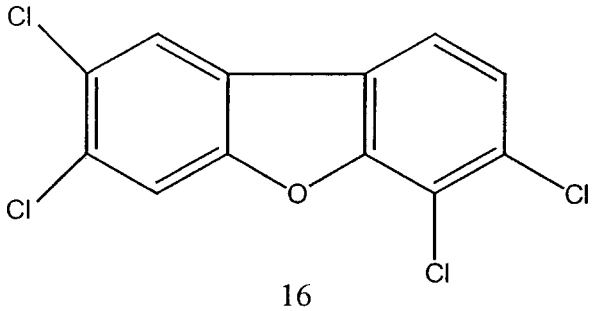
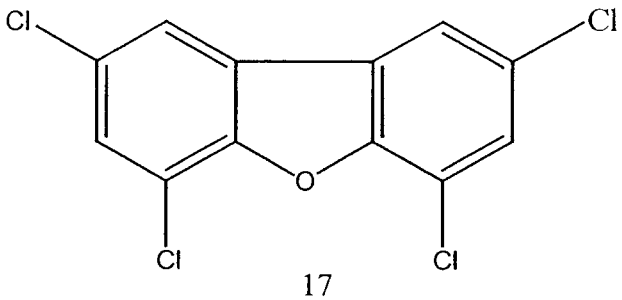


FIG. 1. Structure of compounds calculated in this article. H atoms are not shown.



16

2.3.6.7 - Tetrachlorodibenzofuran



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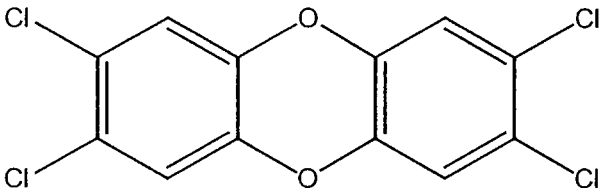
2,4,6,8 -Tetrachlorodibenzofuran



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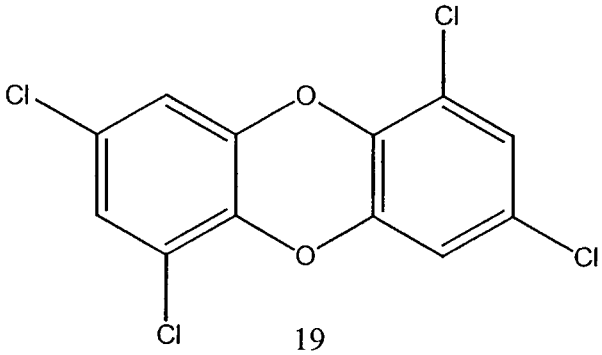
2,3,7,8-Tetrachlorodibenzo-*p*-dioxin



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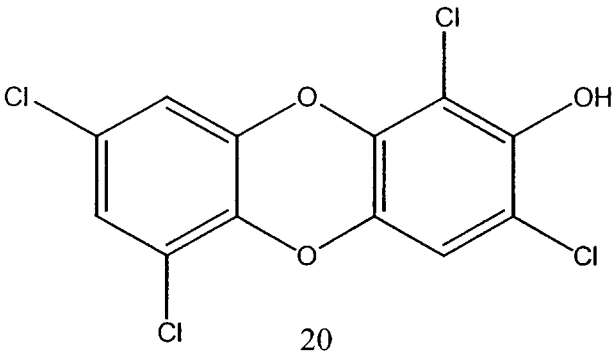
1,3,6,8 Tetrachlorodibenzo-*p*-dioxin



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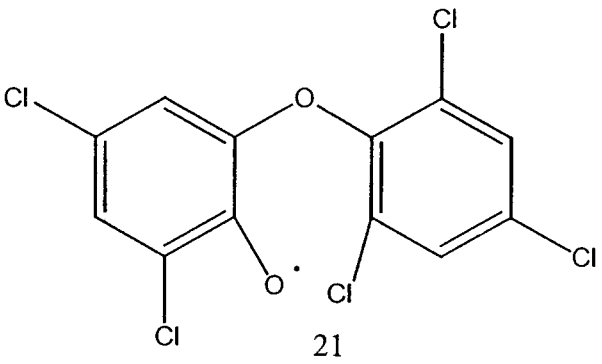
1,3,6,8 Tetrachlorodibenzo-*p*-dioxin-2-ol



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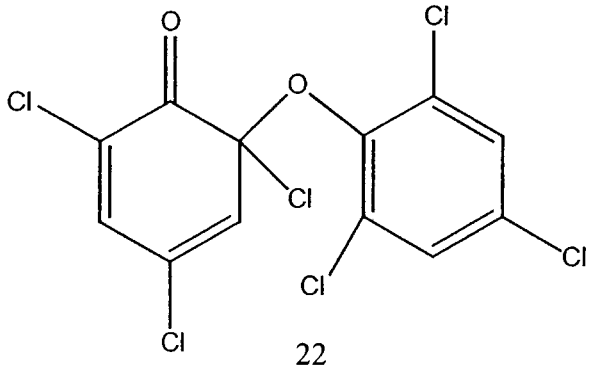
2,4-Dichlorophenoxy-1',3',5'-trichlorophenyl-6-2' Ether Radical



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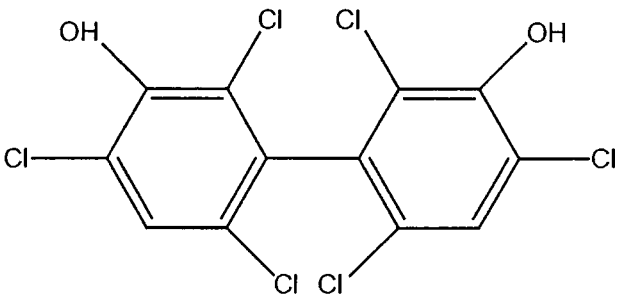
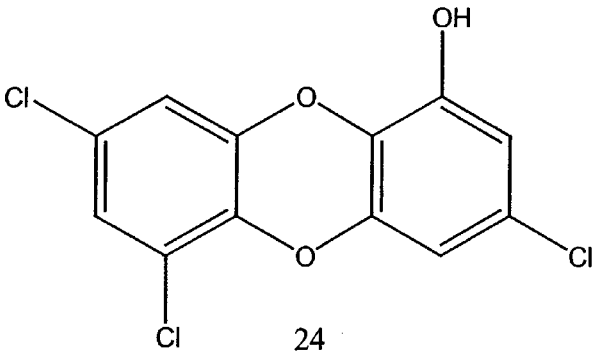


23

2,4,6-2',4',6'-Hexachloro-biphenyl-3,3'-diol

FIG. 1. (Continued.)



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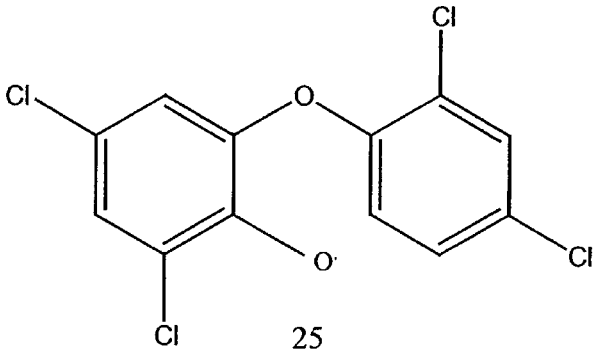
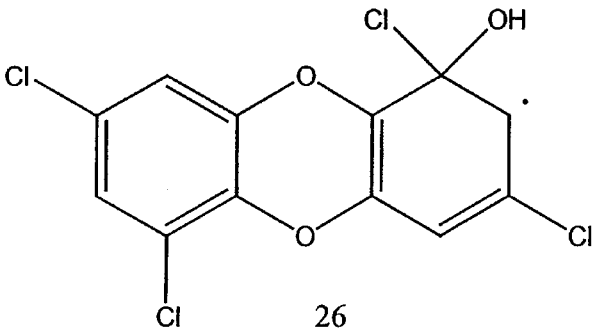
2,4,7-Trichlorodibenzo-*p*-dioxin-9-ol



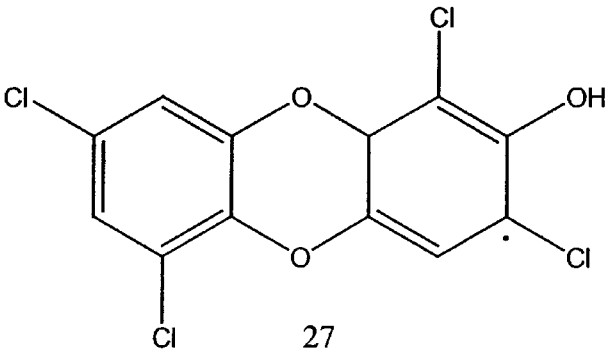
25

2,4-Dichlorophenoxy-1',3'-Dichlorophenyl 6,6'-Ether Radical



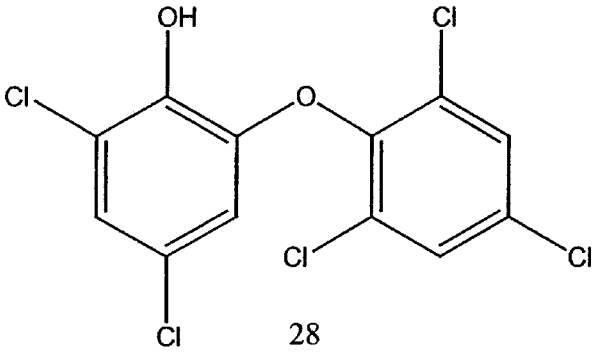
26

1,3-dichloro-1-ol-2-yl-3,5-hexadiene-p-Dioxin-6-8-dichlorobenzen Radical



27

1,3-dichloro-2-ol-3-yl-1,4,hexadiene-p-Dioxin-6,8-dichlorobenzene



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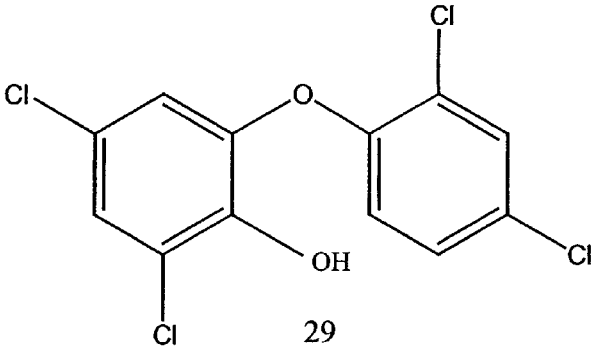
2,4-dichlorophenol-1',3',5'-trichlorophenyl -6-6'-ether



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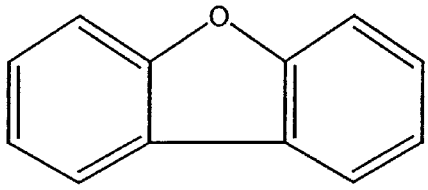
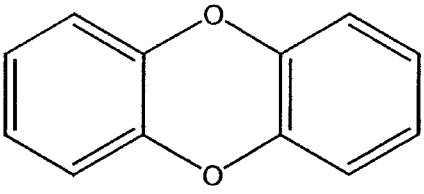
2,4-Dichlorophenoxy-1',5'-Dichlorophenyl 6,2'-Ether



30

Dibenzofuran



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Dibenzo-*p*-dioxin

FIG. 1. (Continued.)

1. $C_5H_2Cl_2O$	3,4-dichloro-2,4-cyclopentadiene-1-one
2. $\cdot C_5H_2Cl_3$	trichloro-1,3,4-cyclopentadienyl radical
3. $C_5H_3Cl_3O$	1-hydroxy-1,3,4-trichlorocyclopentadiene
4. $C_6H_2Cl_3O\cdot$	2,4,6-trichlorophenoxy radical (P·)
5. $\cdot C_6HCl_3OH$	2,4,6-trichlorophenol-3-yl radical
6. $C_6H_2Cl_3O_3\cdot$	2,4,6-trichlorobicyclo-2,5-hexadiene-1,4-peroxy-1-phenoxy radical
7. $C_6H_2Cl_3O_3\cdot$	2,4,6-trichlorobicyclo-2-hexene-1-one-4,6-peroxy-5-yl radical
8. $C_6H_3Cl_3O$	2,4,6-trichlorophenol (P)
9. $C_6H_3Cl_3O_2$	2-hydroxy-2,4,6-trichloro-3,5-cyclohexadiene-1-one
10. $C_6H_4ClO\cdot$	o-chlorophenoxy radical
11. $\cdot C_6H_4ClO$	2,5-cyclohexadiene-2-chloro-1-one-4-yl
12. $\cdot C_6H_4ClO$	2,4-cyclohexadiene-6-chloro-1-one-2-yl radical
13. $C_6H_4Cl_2O$	2,4-dichlorophenol
14. C_6H_5ClO	o-chlorophenol
15. $\cdot C_6H_5O$	2,4-cyclohexadiene-1-one-2-yl radical
16. $C_{12}H_4OCl_4$	2,3,6,7-tetrachlorodibenzofuran
17. $C_{12}H_4OCl_4$	2,4,6,8-tetrachlorodibenzofuran
18. $C_{12}H_4O_2Cl_4$	2,3,7,8-tetrachlorodibenzo-*p*-dioxin
19. $C_{12}H_4O_2Cl_4$	1,3,6,8-tetrachlorodibenzo-*p*-dioxin
20. $C_{12}H_4Cl_4O_3$	1,3,6,8-tetrachlorodibenzo-*p*-dioxin-2-ol
21. $C_{12}H_4Cl_5O_2\cdot$	2,4-dichlorophenoxy-1′,3′,5′-trichlorophenyl-6-6′ ether radical (PD·)
22. $C_{12}H_4Cl_6O_2$	2,4,6-trichlorocyclohexa-3,5-diene-1-one-1′,3′,5′-trichloro-phenyl-2-6′ -ether (PP)
23. $C_{12}H_4Cl_6O_2$ or $C_6HCl_3OH-C_6HCl_3OH$	2,4,6,2′,4′,6′-hexachloro-biphenyl-3,3′-diol
24. $C_{12}H_5Cl_3O_3$	2,4,7-trichlorodibenzo-*p*-dioxin-9-ol
25. $C_{12}H_5Cl_4O_2\cdot$	2,4-dichlorophenoxy-1′,3′ dichlorophenyl 6-6′-ether radical
26. $C_{12}H_5Cl_4O_3\cdot$	1,3-dichloro-1-ol-2-yl-3,5,-cyclohexadiene-*p*-dioxin-6,8-dichlorobenzen radical
27. $\cdot C_{12}H_5Cl_4O_3$	1,3-dichloro-2-ol-3-yl-1,4-cyclohexadiene-p-dioxin-6,8-dichlorobenzene radical
28. $C_{12}H_5Cl_5O_2$	2,4-dichlorophenol-1′,3′,5′-trichlorophenyl-6-6′ ether (PD)
29. $C_{12}H_6Cl_4O_2$	2,4-dichlorophenol-1′,3′-dichlorophenyl-6-2′-ether
30. $C_{12}H_8O$	dibenzofuran (DF)
31. $C_{12}H_8O_2$	dibenzo-*p*-dioxin (DD)

Every available relevant experimental parameter such as infrared (IR) spectra (NIST Chemistry WebBook[26]) and experimental enthalpies of formation, were gathered in order to calculate the thermodynamic properties of these species. If experimental or proposed parameters were not located in the archived literature, the molecular properties were calculated using the MOPAC program (Stewart[27]) and in two cases (6 and 7) using GAUSSIAN 98 with the HF method. It has been shown (Burcat[28] and Curran *et al.*[29]) that MOPAC's calculated vibrations and moments of inertia compare well with calculations resulting from different Gaussian basis sets, as well as with experimental IR spectrum for large molecules. Therefore the MOPAC calculated spectrum and molecular geometry can be used with confidence.

On the other hand, the size of these molecules and the number of ''heavy'' atoms included, prohibited us from using an *ab initio* program for all the molecules because the expected calculation time for each specie would have necessitated a lot of parallel computer time. Thus the use of *ab initio* methods is currently impractical for large models.

2. Enthalpies of Formation

It has been found in practice that while MOPAC and other *ab initio* programs give results regarding the fundamental vibrations of the molecules in close relation to one another, the predictions of the enthalpy of formation can differ up to a factor of 2. The mean absolute error of the AM1 method was reported to be 50.2 kJ mol^{-1} (12 kcal mol^{-1}).[27,30,31] For PM3 this absolute error is smaller for chlorinated compounds. STO/3-21G calculations performed for some of the species gave unacceptable results.

It is found that Benson's group additivity method (Benson[32]) is far more reliable than any other estimate. But even this method does not give uniform answers since there are disputes among different groups of researchers regarding specific values of some of the groups, while other groups are missing.

3. MOPAC Calculations

3.1. Stable Molecules

These are easier to calculate. All the electrons in these molecules are paired, and therefore calculating restricted Hartree–Fock (RHF) conditions and unrestricted Hartree–Fock (UHF) for the same semi empirical method PM3 or AM1 should give the same result. Thus the spin contamination should be zero. All deviations imply higher uncertainties of the calculated data. The PM3 is better adjusted to handle molecules including oxygen and chlorine (Stewart[30]). The AM1 method is supposedly better adjusted for compounds including carbon and hydrogen only. Therefore it is less suitable for our purposes as seen in the individual results. Neither AM1 nor PM3 are adjusted for polyaromatic molecules (Stewart[27]). Therefore the present research can be used for evaluating the two methods for chlorophenols and PCDD derivatives.

During the revision of this article, the CHEM3D-MOPAC-2000[40] package became available for the analysis of spectral data as well. The automatic graphical interface made it possible to recheck all the species and to ascertain that the configurations calculated in the first round were correct. As a rule the data obtained using MOPAC-2000 versus MOPAC 6 were identical to within 0.5%.

3.2. Radicals

All the radicals have unpaired electrons and therefore the calculations may have spin contamination. These were not found to be excessive for most radicals.

4. Thermodynamic Calculations

The thermodynamic calculations were made with the McBride and Gordon[33] PAC99 thermodynamic program. The rigid rotor harmonic oscillator approximation (RRHO) was used as is customary for all polyatomic species. The input for this program includes: molecular vibrations, moments of inertia, and the enthalpy of formation at 298 K. Where needed, the calculated fundamentals were supplemented with internal rotation information calculated using the PM3 calculated Cartesian coordinates and Wang's program.[34] All these data are presented in individual tables for each specie.

In each case the experimental inputs were preferred if they existed. Thus the IR spectrum was used and the missing vibrations were obtained from PM3 calculations. If no IR spectra were available, then the PM3 vibrations were accepted, and the moments of inertia were preferred from PM3. For the enthalpies of formation, since experimental values do not exist, estimations were initiated. These data are presented in calories as they are found in the literature or as given by the semiempirical programs.

The results of the thermodynamic calculations are presented for each species in a table where C_p, the heat capacity; $H°(T)-H°(298.15\ \mathrm{K})$, the enthalpy; $S°$, the entropy; $-[G°-H°(298.15\ \mathrm{K}))/T]$; $H(T)$, the absolute enthalpy; $\Delta_f H°(T)$, the enthalpy of formation; and K_p, the equilibrium constant; are presented as functions of T. $H(T)$, known as "absolute enthalpy," is a function used in engineering and is equal to

$$H(T)=\Delta_f H°(298.15\ \ K)+[H°(T)-H°(298.15\ \ K)].$$

The results are presented in Joules.

5. Accuracy of Calculations

Although the IR spectra were not fully assigned and analyzed spectroscopically, the MOPAC calculated vibrations give values very close to the spectral peaks. Indeed it was found that the main differences between data calculated with IR vibrations and data calculated with MOPAC vibrations results in the entropy values, of the order of up to $8.4\ \mathrm{J\ K^{-1}\ mol^{-1}}$. That is caused mainly by taking into account different internal rotations with different rotational barrier values, rather than differences in the vibration values due to improper assignment.

Table 1 presents comparison of the present C_p and S data with the data that can be estimated with the NIST 94 program (Stein)[35] (Benson's method and data), with Shaub's data[36] for the few available compounds, and with the Thergas[37] estimation, which is a combination of Benson's method and additions like Yoneda.[61] The NIST program does not include any corrections for the Cl–Cl interactions as well as Cl–OH interactions. It also cannot differentiate between different isomers such as the three *o-m-p*-chlorophenols. Although Thergas[37] is a little more sophisticated than NIST 94[35] and THERM,[38] it also cannot differentiate even among very different isomers such as species 9 and 10. Therefore this program (Thergas)[37] is not very different from the previous two, and definitely cannot serve, in its present form, as a universal black box thermodynamic estimator as the authors try to hint and as some researchers unknowingly claimed.

The estimates of THERM[38] cannot be shown together with other programs, because THERM as opposed to the other two is an open-end program, where one is free to use any groups in any number and there are no restrictions imposed by the program. If compared on a one to one basis to NIST 94,[35] the differences will be only due to changes in the values of some molecular groups as calculated by Bozzelli *et al.*, or others.

In the case of dibenzofuran, dibenzo-*p*-dioxin and their tetrachloro compounds where we have used the DFT-B3LYP calculations supplied to us by Dorofeeva[48] we compare those data with our PM3 calculations, although the thermodynamic tables were calculated according to Dorofeeva's data and not PM3.

It is worth noticing that the big discrepancies between the PM3 calculations (or the *ab initio* in some instances) and the ones based on group additivity, appear at molecules that have internal rotations like molecule 23.

TABLE 1. Comparison of the thermodynamic data with the literature (units are cal K^{-1} mol^{-1})

Compound	T/K	NIST[a] 25[35] C_p	NIST[a] 25[35] S	Shaub[36] C_p	Shaub[36] S	Thergas[37] C_p	Thergas[37] S	This study PM3 C_p	This study PM3 S
4. $C_6H_2Cl_3O$	300					33.74	95.25	**34.08**	**98.34**
	1000					57.25	153.55	**57.83**	**154.83**
5. $C_6H_2Cl_3O$	300	36.2	102.9			34.66	96.75	**34.84**	**94.91**
	1000	57.7	—			57.65	154.56	**60.35**	**152.98**
6. $C_6H_2Cl_3O_3$	300					44.77[a]	106.50[a]	**39.58**	**101.77**
2,5 cy-hexadiene	1000					71.12	178.89	**68.74**	**168.92**
7. $C_6H_2Cl_3O_3$	300					40.38[a]	103.04[a]	**40.39**	**103.77**
2-cyclohexene	1000					69.21	171.12	**68.74**	**171.33**
8. $C_6H_3Cl_3O$	300	36.9	97.3	35.98	94.21	35.74	94.39	**34.83**	**94.71**
	1000	61.5	—	62.03	154.37	61.53	155.21	**60.35**	**152.98**
9. $C_6H_2Cl_3O$	300					39.37	109.94	**33.66**	**104.20**
	1000					85.5	182.04	**57.34**	**159.67**
10. $C_6H_2Cl_3O$	300					39.37	109.94	**39.30**	**99.77**
	1000					85.50	182.04	**66.13**	**164.41**
11. C_6H_4ClO	300					26.16	82.81	**26.28**	**83.53**
	1000					53.26	133.08	**53.77**	**132.38**
14. $C_6H_4Cl_2O$	300	32.7	89.9	32.20	88.61			**31.31**	**87.59**
	1000	59.5	—	60.03	145.01			**58.16**	**142.18**
15. C_6H_5ClO	300	28.6	83.9					**28.55**	**82.12**
	1000	57.6	—					**56.51**	**153.85**
16. $C_{12}H_4Cl_4O$-2367	300					***53.80***[b]	***118.55***[b]	53.37	120.49
	1000					***102.19***	***215.06***	100.84	215.24
17. $C_{12}H_4Cl_4O$-2468	300					***53.91***[b]	***117.89***[b]	53.55	117.66
	1000					***102.22***	***214.46***	100.97	212.55
18. $C_{12}H_4Cl_4O_2$-2378	300					**57.99**[c]	**122.98**[c]	57.12	123.91
	1000					**107.10**	**224.46**	106.27	223.79
19. $C_{12}H_4Cl_4O_2$-1368	300			56.96	114.61	**58.05**[c]	**124.97**[c]	57.17	125.48
	1000			107.08	215.37	**107.08**	**226.43**	106.27	225.40
23. $C_{12}H_4C_{16}O_2$	300	73.9	154.					**68.80**	**137.60**
	1000	118.1	273.7					**115.55**	**250.82**
30. $C_{12}H_8O$	300					***39.36***[b]	***89.94***[b]	38.25	90.00
	1000					***94.21***	***171.57***	93.00	179.71
31. $C_{12}H_8O_2$	300			42.41	92.94	***43.29***[b]	***95.07***[b]	41.85	95.01
	1000			99.55	179.80	***99.63***	***182.37***	98.49	180.31

[a]HF/6-31G(d).
[b]Dorofeeva[48] (*ital*).
[c]Mhin *et al.*[44]
[d]**Bold**: values from tables in this article.

6. Kinetic References

Table 2[17] lists a set of 24 elementary reactions from a mechanism for the formation of TCDD (tetrachlorodibenzodioxin) from 2,4,6 trichlorophenol, which includes many of the species described in this paper. The rate constants given in the table were assembled and estimated using the thermodynamic data calculated in this paper. The complete model included 70 elementary reactions. They were all used with the CHEMKIN program in order to be compared to experimental data and the other reactions and the results were described elsewhere (Khachatryan *et al.*[53]).

7. Individual Species

7.1. $C_5H_2Cl_2O$ (3,4-dichloro-2,4-cyclopentadiene-1-one)

This chloro cyclopentadiene ketone is not listed in any thermodynamic compendium. There are no experimental data and this molecule was never calculated. The moments of inertia of the molecule were taken from the PM3 calculation, as were the molecular vibrations.

Only a very rough estimation of the enthalpy of formation could be done with the THERM[38] program, and these ranged from -95 to -52.3 kJ mol^{-1} (-22.7 to -12.5 kcal mol^{-1}). We have chosen the value of -58.6 ± 50.2 kJ mol^{-1} (-14.0 ± 12.0 kcal mol^{-1}) because it involved the smallest number of assumptions (see Tables 3 and 4).

7.2. $\cdot C_5H_2Cl_3$ (trichloro-1,3,4-cyclopentadienyl radical)

There are no literature sources for this species. This is the first calculation of the symmetric trichloro pentadienyl radical. MOPAC calculations were performed and the enthalpy of formation could be estimated only with the Thergas program[37] using Benson's method.[32] This value is also the average of the four MOPAC calculations (see Tables 5 and 6).

TABLE 2. Kinetic model of formation of chlorinated dioxins in incinerator conditions†

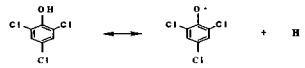
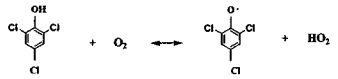
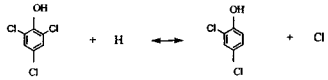
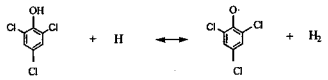
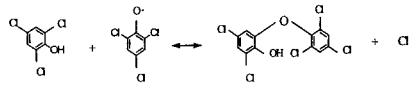
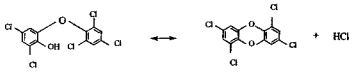
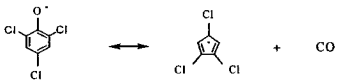
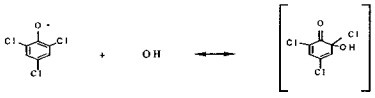
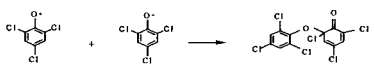
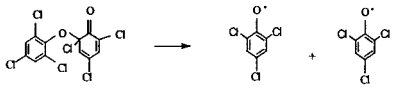
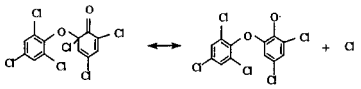
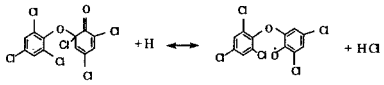
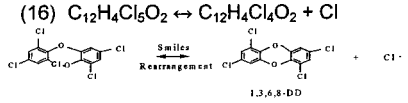
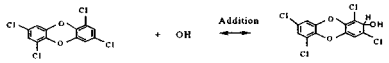
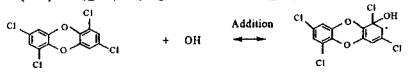
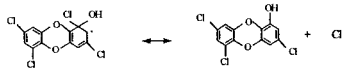
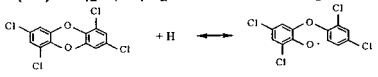
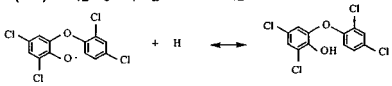
Reaction	A	N	E_a cal/mol	$\Delta_r H$ (298) kcal/mol	Ref
(1) $C_6H_3Cl_3O \leftrightarrow C_6H_2Cl_3O + H$ 	3.2E+15	0	86500	85.8	20
surface (1') $C_6H_3Cl_3O \leftrightarrow C_6H_2Cl_3O + H$	3.2E+13	0	66500	-	a
(2) $C_6H_3Cl_3O + O_2 \leftrightarrow C_6H_2Cl_3O + HO_2$ 	2.0E+12	0	41400	44.3	53
(3) $C_6H_3Cl_3O + H \leftrightarrow C_6H_4Cl_2O + Cl$ 	1.50E+13	0	7500	-19.2	38
(4) $C_6H_3Cl_3O + H \leftrightarrow C_6H_2Cl_3O + H_2$ 	1.15E+14	0	12400	-18.4	49*
(5) $C_6H_3Cl_3O + OH \leftrightarrow C_6H_2Cl_3O + H_2O$ 	1.0E+12	0	0	-33.5	20
(6) $C_6H_3Cl_3O + Cl \leftrightarrow C_6H_2Cl_3O + HCl$ 	1.43E+14	0	0	-17.3	49*
(7) $C_6H_3Cl_3O + O \leftrightarrow C_6H_2Cl_3O + OH$ 	1.26E+13	0	2891	16.4	49*
(8) $C_6H_3Cl_3O + C_6H_2Cl_3O \leftrightarrow C_{12}H_5Cl_5O_2 + Cl$ 	1.0E+12	0	26000	18.4	20
(9) $C_{12}H_5Cl_5O_2 \leftrightarrow C_{12}H_4Cl_4O_2 + HCl$ 	1.0E+14	0	45000	-3.6	20
(10) $C_6H_2Cl_3O \leftrightarrow C_5H_2Cl_3 + CO$ 	2.50E+12	0	45000	18.3	53
(11) $C_6H_2Cl_3O + OH \leftrightarrow C_6H_3Cl_3O_2$ 	1.0E+12	0	0	-64.6	20

TABLE 2. Kinetic model of formation of chlorinated dioxins in incinerator conditions—Continued

(12) $2C_6H_2Cl_3O \rightarrow C_{12}H_4Cl_6O_2$ 	8.60E+11	0	-1254	-19.4	50
(13) $C_{12}H_4Cl_6O_2 \rightarrow 2C_6H_2Cl_3O$ 	3.00E+15	0	50600	19.4	b
(14) $C_{12}H_4Cl_6O_2 \leftrightarrow C_{12}H_4Cl_5O_2 + Cl$ 	1.00E+15	0	48500	33.3	c
(15) $C_{12}H_4Cl_6O_2 + H \leftrightarrow C_{12}H_4Cl_5O_2 + HCl$ 	1.50E+13	0	9500	-69.78	d
(16) $C_{12}H_4Cl_5O_2 \leftrightarrow C_{12}H_4Cl_4O_2 + Cl$  1,3,6,8-DD	1.00E+12	0	36500	17.82	e,53
(17) $C_{12}H_4Cl_5O_2 \leftrightarrow C_{12}H_4O_2Cl_4+Cl$  1,3,7,9-DD	1.00E+12	0	36500	17.82	e,53
(18) $C_{12}H_5Cl_5O_2 + OH \leftrightarrow C_{12}H_4Cl_5O_2 + H_2O$ 	1.00E+12	0	0	-38.03	20
(19) $C_{12}H_4Cl_4O_2 + OH \leftrightarrow C_{12}H_5Cl_4O_3$ 	1.20E+12	0	0	-45.0	51
(20) $C_{12}H_5Cl_4O_3 + O_2 \leftrightarrow C_{12}H_4Cl_4O_3 + HO_2$ 	1.00E+12	0	2000	11.3	F
(21) $C_{12}H_4Cl_4O_2 + OH \leftrightarrow C_{12}H_5O_3Cl_4$ 	1.20E+12	0	0	-71.4	51
(22) $C_{12}H_5O_3Cl_4 \leftrightarrow C_{12}H_5Cl_3O_3 + Cl$ 	1.00E+13	0	4000	48.9	g
(23) $C_{12}H_4Cl_4O_2 + H \quad C_{12}H_5Cl_4O_2$ 	1.0E+13	0	7000	-31.2	h
(24) $C_{12}H_5Cl_4O_2 + H \quad C_{12}H_6Cl_4O_2$ 	1.0E+14	0	0	-81.27	I

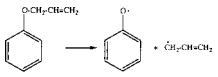
†$k=AT^n \exp(-E_a/RT)$. Units are s^{-1} cm^{-3} mol^{-1} s^{-1} and cm^{-6} mol^{-2} s^{-1} for uni-, bi-, and tri-molecular reactions, respectively; E_a are in cal/mol; and $\Delta_1 H$ in kcal/mol from this study.

*Analogy with the reactions: phenol + H (reaction 4), phenol + CI (reaction 6), phenol + O (reaction 7).

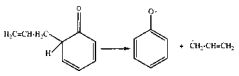
[a]Taking into account that preexponential factors for monomolecular reactions in the absorbed layer are of the order of magnitude $\sim 10^{12}$–10^{13} s^{-1},[55] E_a was empirically adjusted.

TABLE 2. Kinetic model of formation of chlorinated dioxins in incinerator conditions—Continued

[b] For benzyl phenyl ethers and anisole, preexponential factrors of the oxygen–carbon bond fission reactions are usually $\sim 10^{15.2}$ s^{-1}.[56] The rate coefficient for reaction 13 was assigned by analogy with the following reaction[57] which also forms two resonantly stabilized radicals:



[c] By analogy with the reaction



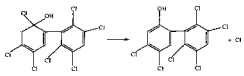
with estimated $k = 10^{15} \exp(-44\,500/RT)$ s^{-1}.[57] $E_a = 48\,500$ cal/mol was adjusted for the chlorinated species involved in this reaction.

[d] Based on typical bimolecular rate constants for Cl abstraction by H; $H + CH_3Cl \rightarrow H_2 + CH_2Cl$ (or $HCl + CH_3$) with $k = 3.7 10^{10} \exp(-4680/RT)$,[58] see also Ref. 54.

[e] The same rate constant parameters (details in Ref. 53) were assigned for reactions 16 and 17 (see also Ref. 59).

[f] By analogy with bulk radical + oxygen reaction, i.e.; $n\text{-}C_7H_{15} + O_2 \rightarrow C_7H_{14} + HO_2$; $k = 10^{12} \exp(-2000/RT)$.[60]

[g] By analogy with the reaction



with $E_a = 4$ kcal/mol calculated in Ref. 63.

[h] By analogy with Cl + PhOPh(diphenyl ether) $\rightarrow$ PhO· + PhCl.[22] In this work, it is suggested that the splitting of PhOPh by Cl, is as fast as hydrogen abstraction with $E_a \sim 6-7$ kcal/mol. We consider the splitting of PCDD by H atoms as a ring opening process and assign $E_a \sim 7$ kcal/mol for this reaction.

[i] Rate coefficient typical for atom–polyatomic radical recombination.[49]

TABLE 3. Molecular properties of $C_5H_2Cl_2O$ (3,4-dichloro-2,4-cyclopentadiene-1-one)

	Enthalpy of formation $\Delta_f H°(298.15\ K)$ / kcal mol^{-1}	Zero point energy ZPE / kcal mol^{-1}
Our estimation	**−14±12**	—
PM3	−0.100	35.613
PM3 UHF	−0.661	34.535
AM1	6.732	37.176
AM1 UHF	5.879	36.177

	Principal moments of inertia / g $cm^2 \times 10^{-39}$		
MOPAC method	I_a	I_b	I_c
PM3	**41.601 251 9**	**71.066 249 7**	**112.675 015**
PM3 UHF	41.601 251 9	71.066 249 7	112.675 015
AM1	41.601 251 9	71.066 249 7	112.675 015
AM1 UHF	41.601 251 9	71.066 249 7	112.675 015

	Molecular vibrations / cm^{-1}					
AM1	141.8	152	173.8	305	362	477
	534	552	646	691	798	870
	959	1036	1089	1186	1233	1269
	1371	1758	1763	2130	3252	3257
AM1 UHF	136.5	139.3	173	303	327	477
	530	548	628	653	781	837
	923	1028	1084	1185	1207	1264
	1271	1533	1640	2129	3251	3255
PM3	**151.4**	**163**	**188**	**297**	**370**	**410**
	458	**547**	**654**	**669**	**711**	**876**
	940	**957**	**978**	**1146**	**1147**	**1255**
	1301	**1725**	**1743**	**1951**	**3137**	**3141**
PM3 UHF	151.2	152.2	184	295	340	410
	455	543	639	640	693	844
	925	934	971	1118	1145	1212
	1250	1423	1610	1949	3135	3137

TABLE 4. Thermodynamic properties of $C_5H_2Cl_2O$ (3,4-dichlorocyclopentadiene-1-one) ($M_r = 148.976$)

Enthalpy Reference Temperature = T_r = 298.15 K				Standard State Pressure = $p°$ = 0.1 MPa			
T (K)	C_p° ($J\cdot K^{-1}\cdot mol^{-1}$)	$H°-H°(T_r)$ ($J\cdot mol^{-1}$)	$S°$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$-[G°-H°(T_r)]/T$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$H(T)$ ($kJ\cdot mol^{-1}$)	$\Delta_f H°$ ($kJ\cdot mol^{-1}$)	log K_f
0	—	−20.365	—	—	−78.941	−51.685	—
100	53.953	−16.343	262.516	425.951	−74.919	−55.331	22.7079
200	83.213	−9.463	309.044	356.359	−68.039	−57.273	8.0394
298.15	109.022	0.000	347.197	347.197	−58.576	−58.576	3.0637
300	109.471	0.202	347.873	347.199	−58.374	−58.596	3.0005
400	131.395	12.285	382.481	351.769	−46.291	−59.492	0.4310
500	148.784	26.329	413.747	361.090	−32.247	−60.104	−1.1307
600	162.405	41.916	442.128	372.268	−16.660	−60.545	−2.1808
700	173.153	58.714	468.002	384.124	0.138	−60.846	−2.9357
800	181.751	76.475	491.705	396.111	17.899	−61.014	−3.5042
900	188.726	95.011	513.529	407.961	36.435	−61.048	−3.9470
1000	194.454	114.179	533.719	419.540	55.603	−60.973	−4.3011
1100	199.206	133.869	552.482	430.783	75.293	−60.798	−4.5903
1200	203.184	153.994	569.991	441.663	95.418	−60.543	−4.8304
1300	206.539	174.485	586.391	452.171	115.909	−60.229	−5.0328
1400	209.388	195.285	601.804	462.314	136.709	−59.884	−5.2049
1500	211.823	216.349	616.335	472.103	157.773	−59.505	−5.3537
1600	213.917	237.638	630.075	481.551	179.062	−59.123	−5.4829
1700	215.727	259.123	643.099	490.674	200.547	−58.748	−5.5961
1800	217.301	280.776	655.475	499.488	222.200	−58.389	−5.6961
1900	218.676	302.576	667.262	508.011	244.000	−58.056	−5.7850
2000	219.883	324.506	678.509	516.257	265.930	−57.756	−5.8643
2100	220.947	346.548	689.264	524.241	287.972	−57.497	−5.9361
2200	221.889	368.691	699.565	531.978	310.115	−57.293	−6.0009
2300	222.726	390.922	709.447	539.480	332.346	−57.139	−6.0600
2400	223.474	413.233	718.942	546.761	354.657	−57.048	−6.1143
2500	224.144	435.615	728.078	553.833	377.039	−57.033	−6.1637
2600	224.745	458.060	736.881	560.705	399.484	−57.083	−6.2095
2700	225.288	480.562	745.374	567.388	421.986	−57.216	−6.2521
2800	225.779	503.115	753.576	573.892	444.539	−57.432	−6.2919
2900	226.224	525.716	761.507	580.225	467.140	−57.733	−6.3287
3000	226.629	548.359	769.183	586.397	489.783	−58.135	−6.3633
3100	226.999	571.041	776.620	592.414	512.465	−58.617	−6.3963
3200	227.337	593.758	783.833	598.283	535.182	−59.201	−6.4274
3300	227.647	616.507	790.833	604.013	557.931	−59.880	−6.4567
3400	227.931	639.286	797.633	609.608	580.710	−60.655	−6.4847
3500	228.193	662.093	804.244	615.075	603.517	−61.532	−6.5117
3600	228.435	684.924	810.676	620.419	626.348	−62.498	−6.5373
3700	228.658	707.779	816.938	625.646	649.203	−63.563	−6.5621
3800	228.865	730.655	823.039	630.761	672.079	−64.720	−6.5858
3900	229.057	753.552	828.986	635.768	694.976	−65.964	−6.6089
4000	229.236	776.466	834.788	640.671	717.890	−67.305	−6.6310
4100	229.402	799.398	840.450	645.475	740.822	−68.717	−6.6529
4200	229.557	822.346	845.980	650.183	763.770	−70.215	−6.6740
4300	229.702	845.309	851.383	654.800	786.733	−71.795	−6.6943
4400	229.837	868.286	856.666	659.328	809.710	−73.462	−6.7142
4500	229.964	891.276	861.832	663.771	832.700	−75.183	−6.7338
4600	230.083	914.279	866.888	668.132	855.703	−76.967	−6.7530
4700	230.194	937.293	871.837	672.413	878.717	−78.806	−6.7718
4800	230.299	960.317	876.685	676.619	901.741	−80.699	−6.7904
4900	230.398	983.352	881.434	680.750	924.776	−82.641	−6.8087
5000	230.491	1006.397	886.090	684.811	947.821	−84.681	−6.8263
5100	230.579	1029.450	890.655	688.802	970.874	−86.705	−6.8442
5200	230.662	1052.513	895.133	692.727	993.937	−88.804	−6.8615
5300	230.741	1075.583	899.528	696.588	1017.007	−90.943	−6.8785
5400	230.815	1098.661	903.842	700.386	1040.085	−93.121	−6.8953
5500	230.885	1121.746	908.077	704.124	1063.170	−95.333	−6.9119
5600	230.952	1144.838	912.238	707.803	1086.262	−97.579	−6.9282
5700	231.015	1167.936	916.327	711.426	1109.360	−99.855	−6.9444
5800	231.076	1191.041	920.345	714.993	1132.465	−102.161	−6.9604
5900	231.133	1214.151	924.295	718.507	1155.575	−104.495	−6.9761
6000	231.187	1237.267	928.181	721.969	1178.691	−106.851	−6.9917

TABLE 5. Molecular properties of $\cdot C_5H_2Cl_3$ (trichloro-1,3,4-cyclopentadienyl radical)

	Enthalpy of formation $\Delta_f H°(298.15\ K)$ / kcal mol^{-1}	Zero point energy ZPE / kcal mol^{-1}
Our estimate	**36.9±5**	—
Thergas[15]	36.98	
PM3	39.08	33.081
PM3 UHF	32.44	32.834
AM1	41.83	34.397
AM1 UHF	34.30	34.298

Moments of inertia of the molecule / g cm^2×10^{-39}

MOPAC method	I_a	I_b	I_c
PM3	**41.150 8**	**112.3192**	**153.4698**
PM3 UHF	41.324 45	112.8528	154.1773
AM1	42.339 65	115.1571	157.4967
AM1 UHF	42.472 84	115.5446	158.0175

Molecular vibrations / cm^{-1}

AM1	123.2	154.6	168.7	208	355	393
	463	480	569	663	728	816
	880	901	1009	1125	1151	1210
	1402	1474	1626	1652	3263	3269
AM1 UHF	120.7	143.6	168	206	329	432
	449	486	541	616	723	859
	872	1000	1015	1122	1193	1217
	1390	1465	1526	1579	3260	3266
PM3	**118.3**	**145.3**	**146.8**	**200**	**336**	**358**
	387	**453**	**554**	**629**	**634**	**864**
	893	**899**	**939**	**1029**	**1035**	**1153**
	1378	**1439**	**1623**	**1635**	**3140**	**3166**
PM3 UHF	117.4	141.7	148	198	320	381
	402	454	528	595	629	845
	866	924	963	1032	1086	1164
	1349	1428	1527	1561	3146	3151

7.3. $C_5H_3Cl_3O$ (1-hydroxy-1,3,4-trichlorocyclopentadiene)

This molecule is not mentioned in the literature. The MOPAC PM3 data were used for the thermodynamic calculation and the enthalpy of formation was estimated as the average of PM3 and PM3-UHF. The calculation of AM1 UHF failed. The reduced moment of inertia was calculated with a program by Wang[34] (see Tables 7 and 8).

7.4. $C_6H_2Cl_3O\cdot$ (2,4,6-trichlorophenoxy radical) (P·)

This is an oxygen centered radical. Experimental as well as other molecular information regarding this radical, which belongs to the group of polychlorinated phenol compounds denoted in short as (P·), is not available in the literature. It was calculated using the MOPAC methods and the PM3 values were preferred.

The enthalpy of formation is very roughly estimated using the NIST 94[35] approximation and adding the Dorofeeva *et al.*[39] Cl–Cl corrections. The value obtained is $\Delta_f H°(298.15\ K) = -32.64 \pm 12.5\ kJ\ mol^{-1}$ [$\Delta_f H° \times (298.15\ K) = -7.8 \pm 3\ kcal\ mol^{-1}$] (see Tables 9 and 10).

7.5. $\cdot C_6HCl_3OH$ (2,4,6-trichlorophenol-3-yl radical)

This is a carbon centered radical with the electron localized on the benzene ring. No experimental or other values were available. This radical was calculated using the MOPAC PM3 method.

The enthalpy of formation is a very rough approximation using the NIST 94[35] and the THERM[38] programs together with the PM3 calculations (see Tables 11 and 12).

7.6. $C_6H_2Cl_3O_3\cdot$ (2,4,6-trichlorobicyclo-2,5-hexadiene-1,4-peroxy-1-phenoxy radical)

No experimental or other values are available for this species. This bicyclo symmetric radical was calculated using the GAUSSIAN 98 HF/6-31G(d) and MOPAC PM3 method. Because it is symmetric the two possible conformations (O–O bridge above or below the phenyl ring) are equivalent. The unscaled *ab initio* calculations compare well with the MOPAC PM3 results (see Table 13). However since for the next similar radical (7.7), only the scaled *ab initio* calculation compared

TABLE 6. Thermodynamic properties of $\cdot C_5H_2Cl_3$ (trichloro-1,3,4-cyclopentadienyl radical) ($M_r = 168.429$)

Enthalpy Reference Temperature = T_r = 298.15 K				Standard State Pressure = $p°$ = 0.1 MPa			
T (K)	C_p° ($J\cdot K^{-1}\cdot mol^{-1}$)	$H°-H°(T_r)$ ($J\cdot mol^{-1}$)	$S°$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$-[G°-H°(T_r)]/T$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$H(T)$ ($kJ\cdot mol^{-1}$)	$\Delta_f H°$ ($kJ\cdot mol^{-1}$)	log K_f
0	—	−22.181	—	—	132.208	159.715	—
100	60.559	−17.824	278.187	456.425	136.566	156.399	−87.4774
200	90.863	−10.209	329.763	380.808	144.181	155.128	−46.7808
298.15	116.529	0.000	370.953	370.953	154.390	154.390	−33.4735
300	116.974	0.216	371.675	370.955	154.606	154.379	−33.3067
400	138.596	13.035	408.404	375.816	167.424	153.970	−26.5960
500	155.522	27.777	441.231	385.676	182.167	153.800	−22.5773
600	168.535	44.009	470.788	397.440	198.398	153.768	−19.8998
700	178.614	61.387	497.556	409.861	215.777	153.838	−17.9871
800	186.558	79.661	521.946	422.370	234.050	154.002	−16.5516
900	192.935	98.646	544.300	434.693	253.036	154.261	−15.4336
1000	198.137	118.209	564.906	446.698	272.598	154.593	−14.5374
1100	202.435	138.244	583.999	458.322	292.633	154.993	−13.8024
1200	206.025	158.672	601.771	469.545	313.062	155.445	−13.1882
1300	209.049	179.430	618.385	480.362	333.820	155.932	−12.6672
1400	211.616	200.467	633.973	490.783	354.856	156.431	−12.2186
1500	213.811	221.741	648.650	500.823	376.130	156.945	−11.8293
1600	215.698	243.218	662.511	510.499	397.608	157.450	−11.4872
1700	217.331	264.872	675.638	519.831	419.261	157.937	−11.1844
1800	218.751	286.678	688.101	528.836	441.067	158.397	−10.9144
1900	219.992	308.616	699.962	537.533	463.006	158.825	−10.6721
2000	221.083	330.671	711.275	545.939	485.061	159.213	−10.4533
2100	222.044	352.828	722.085	554.072	507.218	159.556	−10.2553
2200	222.896	375.076	732.435	561.946	529.466	159.838	−10.0746
2300	223.654	397.405	742.360	569.576	551.794	160.063	−9.9095
2400	224.331	419.804	751.893	576.975	574.194	160.221	−9.7582
2500	224.937	442.268	761.063	584.156	596.658	160.296	−9.6185
2600	225.482	464.790	769.896	591.131	619.179	160.299	−9.4896
2700	225.974	487.363	778.416	597.911	641.753	160.211	−9.3705
2800	226.419	509.983	786.642	604.505	664.373	160.031	−9.2600
2900	226.823	532.645	794.594	610.924	687.035	159.755	−9.1569
3000	227.190	555.346	802.290	617.175	709.736	159.368	−9.0610
3100	227.526	578.082	809.745	623.267	732.472	158.889	−8.9718
3200	227.832	600.851	816.974	629.208	755.240	158.297	−8.8883
3300	228.113	623.648	823.989	635.005	778.038	157.598	−8.8101
3400	228.372	646.472	830.803	640.664	800.862	156.792	−8.7368
3500	228.610	669.322	837.426	646.191	823.711	155.871	−8.6684
3600	228.829	692.194	843.870	651.593	846.583	154.851	−8.6038
3700	229.032	715.087	850.142	656.875	869.477	153.722	−8.5435
3800	229.220	738.000	856.252	662.042	892.389	152.493	−8.4864
3900	229.395	760.931	862.209	667.098	915.320	151.170	−8.4330
4000	229.557	783.878	868.019	672.049	938.268	149.744	−8.3825
4100	229.708	806.842	873.689	676.898	961.231	148.243	−8.3352
4200	229.849	829.820	879.226	681.650	984.209	146.654	−8.2905
4300	229.980	852.811	884.636	686.308	1007.201	144.982	−8.2481
4400	230.103	875.815	889.925	690.876	1030.205	143.226	−8.2081
4500	230.219	898.831	895.097	695.357	1053.221	141.419	−8.1706
4600	230.327	921.859	900.158	699.754	1076.248	139.555	−8.1351
4700	230.428	944.897	905.113	704.071	1099.286	137.644	−8.1016
4800	230.524	967.944	909.965	708.310	1122.334	135.688	−8.0702
4900	230.614	991.001	914.719	712.474	1145.391	133.694	−8.0404
5000	230.699	1014.067	919.379	716.566	1168.457	131.615	−8.0119
5100	230.779	1037.141	923.948	720.587	1191.530	129.566	−7.9855
5200	230.854	1060.222	928.430	724.541	1214.612	127.456	−7.9602
5300	230.925	1083.311	932.828	728.430	1237.701	125.325	−7.9362
5400	230.993	1106.407	937.145	732.255	1260.797	123.172	−7.9136
5500	231.057	1129.510	941.385	736.019	1283.899	121.003	−7.8921
5600	231.118	1152.619	945.548	739.724	1307.008	118.821	−7.8717
5700	231.175	1175.733	949.640	743.371	1330.123	116.628	−7.8525
5800	231.230	1198.854	953.661	746.962	1353.243	114.426	−7.8342
5900	231.282	1221.979	957.614	750.499	1376.369	112.218	−7.8169
6000	231.332	1245.110	961.501	753.983	1399.500	110.009	−7.8005

TABLE 7. Molecular properties of $C_5H_3Cl_3O$ (1-hydroxy-1,3,4-trichlorocyclopentadiene)

	Enthalpy of formation $\Delta_f H°(298.15\ K)$ / kcal mol^{-1}	Zero point energy ZPE / kcal mol^{-1}
Our estimate	**−24.0±1**	—
PM3	−23.32	44.062
PM3 UHF	−23.65	43.112
AM1	−18.95	45.324

Moments of inertia of the molecule / g cm$^2\times10^{-39}$

MOPAC method	I_a	I_b	I_c
PM3	**55.896 442**	**128.064 243**	**155.830 073**
PM3 UHF	55.895 903	128.063 541	155.829 073
AM1	55.896 442	128.064 242	155.830 073

Reduced moment of inertia[16] $I_r=$ **0.1424** g cm$^2\times10^{-39}$; $\sigma_{rot}=$ **2**; $V(2)=$ **1116.8** cm^{-1}.

Molecular vibrations / cm^{-1}

AM1	92.9	95	171.5	260	298	312
	335	349	469	481	525	554
	690	723	861	889	961	1052
	1086	1191	1216	1224	1394	1458
	1519	1758	1766	3255	3261	3460
PM3	97	**104.7**	**149.7**	**248**	**281**	**322**
	344	**413**	**425**	**487**	**516**	**590**
	621	**666**	**794**	**892**	**930**	**937**
	991	**1128**	**1143**	**1190**	**1329**	**1345**
	1430	**1727**	**1749**	**3142**	**3146**	**3686**
PM3 UHF	92.7	101.9	149.5	246	279	319
	330	413	419	481	512	588
	615	645	778	863	907	933
	985	1120	1142	1185	1235	1342
	1429	1431	1649	3140	3142	3686

well with the PM3 calculations and HF is not one of the best *ab initio* methods, it was decided to use the PM3 results for the thermodynamic Table 14.

The enthalpy of formation was roughly estimated using Bozzelli's[41] proposal for an 0.83 factor used on the PM3 enthalpy of formation like in similar bicyclo peroxy compounds he used. Other methods failed.

7.7. $C_6H_2Cl_3O_3$· (2,4,6-trichlorobicyclo-2-hexene-1-one-4,6-peroxy-5-yl radical)

This bicyclo asymmetric radical was calculated here for the first time using the MOPAC PM3 method and GAUSSIAN 98 HF/6-31G(d). There are at least two main configurations of this radical. The configuration given here was assumed to have the oxygen bridge below the ring. The other configuration (bridge above the ring) gives results with negligible differences. For example the moments of inertia are $I_a=119.6248$, $I_b=130.9687$, $I_c=223.6886$ g cm$^2\times10^{-39}$ compared to those in Table 15. The vibrations differ also by as much as 0.002–0.2%. Despite the fact that for this radical the *ab initio* scaled calculations were very close to those of PM3, to be consistent with the former radical we have preferred here the PM3 calculation.

Its enthalpy of formation was roughly estimated using Bozzelli's[20] proposal for an 0.83 factor used on the PM3 enthalpy of formation as for similar bicyclo peroxy compounds he described (see Table 16).

7.8. $C_6H_3Cl_3O$ (2,4,6-trichlorophenol) (P)

2,4,6-trichlorophenol, belongs to the group of polychlorophenol compounds denoted in short as (P). It was calculated by Shaub[36] using Benson's group additivity methods. In this calculation the IR spectra[26] was compared with the calculated spectra, and a few PM3 calculated vibrations were supplemented to the existing experimental values.

The enthalpy of formation was taken from the NIST 94[35] estimate and corrected using Dorofeeva's[39] corrections (see Tables 17 and 18).

7.9. $C_6H_3Cl_3O_2$ (2-hydroxy-2,4,6-trichloro-3,5-cyclohexadiene-1-one)

This stable trichloro-cyclohexadiene molecule is calculated here for the first time using the MOPAC PM3 method.

Its enthalpy of formation was estimated as the average value of PM3, PM3-UHF, AM1, and AM1-UHF (see Tables 19 and 20).

TABLE 8. Thermodynamic properties of $C_5H_3Cl_3O$ (1-hydroxy-1,3,4-trichlorocyclopentadiene) ($M_r = 185.436$)

Enthalpy Reference Temperature = T_r = 298.15 K				Standard State Pressure = $p°$ = 0.1 MPa			
T (K)	C_p° ($J\cdot K^{-1}\cdot mol^{-1}$)	$H°-H°(T_r)$ ($J\cdot mol^{-1}$)	$S°$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$-[G°-H°(T_r)]/T$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$H(T)$ ($kJ\cdot mol^{-1}$)	$\Delta_f H°$ ($kJ\cdot mol^{-1}$)	log K_f
0	—	−24.098	—	—	−124.514	−88.433	—
100	59.807	−19.865	279.384	478.039	−120.281	−94.824	36.6505
200	101.954	−11.721	334.147	392.754	−112.137	−98.369	11.4811
298.15	135.629	0.000	381.383	381.383	−100.416	−100.416	2.9403
300	136.192	0.251	382.224	381.386	−100.165	−100.445	2.8318
400	162.924	15.266	425.235	387.069	−85.150	−101.596	−1.5657
500	183.201	32.620	463.875	398.634	−67.796	−102.145	−4.2268
600	198.543	51.742	498.696	412.458	−48.674	−102.332	−6.0070
700	210.360	72.212	530.226	427.066	−28.204	−102.267	−7.2795
800	219.697	93.732	558.949	441.784	−6.684	−102.002	−8.2324
900	227.251	116.092	585.276	456.285	15.676	−101.559	−8.9710
1000	233.482	139.138	609.552	470.414	38.722	−100.976	−9.5588
1100	238.696	162.755	632.057	484.098	62.339	−100.270	−10.0367
1200	243.108	186.851	653.021	497.312	86.435	−99.464	−10.4320
1300	246.873	211.355	672.632	510.052	110.939	−98.584	−10.7638
1400	250.107	236.208	691.049	522.329	135.792	−97.659	−11.0451
1500	252.902	261.362	708.402	534.161	160.946	−96.690	−11.2872
1600	255.330	286.776	724.803	545.568	186.360	−95.709	−11.4967
1700	257.450	312.417	740.348	556.573	212.001	−94.728	−11.6795
1800	259.308	338.257	755.117	567.196	237.841	−93.760	−11.8404
1900	260.943	364.272	769.181	577.460	263.856	−92.814	−11.9829
2000	262.389	390.440	782.604	587.384	290.024	−91.900	−12.1096
2100	263.672	416.744	795.437	596.988	316.328	−91.028	−12.2235
2200	264.814	443.169	807.730	606.290	342.753	−90.215	−12.3259
2300	265.835	469.703	819.525	615.306	369.287	−89.457	−12.4187
2400	266.751	496.333	830.858	624.053	395.917	−88.769	−12.5032
2500	267.574	523.050	841.764	632.545	422.634	−88.167	−12.5800
2600	268.317	549.845	852.274	640.795	449.429	−87.640	−12.6506
2700	268.989	576.711	862.413	648.816	476.295	−87.211	−12.7158
2800	269.598	603.641	872.206	656.621	503.225	−86.879	−12.7760
2900	270.153	630.629	881.677	664.219	530.213	−86.649	−12.8317
3000	270.659	657.670	890.844	671.621	557.254	−86.539	−12.8834
3100	271.122	684.759	899.727	678.837	584.343	−86.527	−12.9323
3200	271.546	711.893	908.341	685.875	611.477	−86.638	−12.9779
3300	271.935	739.067	916.703	692.743	638.651	−86.865	−13.0207
3400	272.294	766.279	924.827	699.450	665.863	−87.207	−13.0611
3500	272.624	793.525	932.725	706.003	693.109	−87.675	−13.0997
3600	272.930	820.803	940.409	712.408	720.387	−88.250	−13.1360
3700	273.213	848.110	947.891	718.672	747.694	−88.944	−13.1709
3800	273.475	875.445	955.181	724.800	775.029	−89.748	−13.2039
3900	273.719	902.805	962.287	730.799	802.389	−90.657	−13.2358
4000	273.945	930.188	969.220	736.673	829.772	−91.679	−13.2662
4100	274.157	957.593	975.987	742.428	857.177	−92.785	−13.2958
4200	274.354	985.019	982.596	748.068	884.603	−93.990	−13.3241
4300	274.538	1012.463	989.054	753.597	912.047	−95.289	−13.3513
4400	274.711	1039.926	995.368	759.021	939.510	−96.682	−13.3775
4500	274.873	1067.405	1001.543	764.342	966.989	−98.137	−13.4033
4600	275.025	1094.900	1007.586	769.564	994.484	−99.660	−13.4282
4700	275.168	1122.410	1013.502	774.692	1021.994	−101.240	−13.4525
4800	275.302	1149.933	1019.297	779.727	1049.517	−102.875	−13.4763
4900	275.428	1177.470	1024.975	784.675	1077.054	−104.559	−13.4995
5000	275.548	1205.019	1030.540	789.537	1104.603	−106.337	−13.5217
5100	275.660	1232.579	1035.998	794.316	1132.163	−108.097	−13.5440
5200	275.767	1260.151	1041.352	799.015	1159.735	−109.925	−13.5654
5300	275.868	1287.733	1046.606	803.637	1187.317	−111.785	−13.5864
5400	275.963	1315.324	1051.763	808.185	1214.908	−113.676	−13.6071
5500	276.053	1342.925	1056.828	812.660	1242.509	−115.591	−13.6272
5600	276.139	1370.535	1061.803	817.064	1270.119	−117.527	−13.6470
5700	276.220	1398.153	1066.691	821.401	1297.737	−119.482	−13.6664
5800	276.298	1425.779	1071.495	825.672	1325.363	−121.453	−13.6854
5900	276.371	1453.412	1076.219	829.878	1352.996	−123.437	−13.7040
6000	276.441	1481.053	1080.865	834.023	1380.637	−125.428	−13.7224

TABLE 9. Molecular properties of $C_6H_2Cl_3O\cdot$ (2,4,6-trichlorophenoxy radical). Values listed with bold characters were chosen for thermodynamic calculations—$\sigma = \mathbf{2}$ and statistical weight $= \mathbf{2}$

	Enthalpy of formation $\Delta_f H°(298.15\ \mathrm{K})$ / kcal mol^{-1}	Zero point energy ZPE / kcal mol^{-1}
Our estimate	**−7.8±3.0**	—
NIST 94[35]	−9.9	
PM3	−7.0	39.742
PM3 UHF	−17.04	39.412
AM1	−2.70	41.919
AM1 UHF	−13.74	41.401

Moments of inertia of the molecule / g cm$^2\times10^{-39}$

MOPAC method	I_a	I_b	I_c
PM3	**99.122 034**	**111.076 65**	**210.198 68**
PM3 UHF	99.122 034	111.076 65	210.198 68
AM1	99.122 034	111.076 65	210.198 68
AM1 UHF	99.122 034	111.076 65	210.198 68

Molecular vibrations / cm^{-1}

AM1	46.4	130.5	172.6	199.1	210	336
	342	388	437	453	511	553
	623	789	853	900	944	946
	963	1160	1244	1287	1317	1419
	1466	1640	1677	1974	3159	3162
AM1 UHF	47.4	126.4	158.9	197.7	209	331
	335	386	434	453	484	521
	620	762	849	897	902	902
	956	1157	1247	1281	1418	1451
	1477	1576	1589	1859	3165	3168
PM3	**56.2**	**128.2**	**173.6**	**188**	**191**	**300**
	328	**354**	**377**	**408**	**491**	**539**
	589	**736**	**774**	**778**	**882**	**922**
	936	**1053**	**1144**	**1162**	**1256**	**1371**
	1396	**1625**	**1666**	**1883**	**3045**	**3048**
PM3 UHF	48.3	117.6	149.5	187	191	299
	300	354	376	413	454	504
	584	739	754	771	875	884
	895	1045	1145	1153	1374	1383
	1458	1583	1625	1823	3043	3045

7.10. $C_6H_4ClO\cdot$ (o-chlorophenoxy radical)

There are no experimental data for this oxygen centered radical, and it is not listed in Shaub's[36] and Bozzelli's calculations. Melius calculated the o-chlorophenyl radical (A72N) in his database (Burcat[42]). This radical was calculated using MOPAC, and the enthalpy of formation was estimated using the NIST 94[35] program (see Tables 21 and 22).

7.11. $\cdot C_6H_4ClO$ (2,5-cyclohexadiene-2-chloro-1-one-4-yl)

This radical is calculated here for the first time. The MOPAC PM3 method was used for the thermodynamic calculations.

The enthalpy of formation was roughly estimated using the THERM program (Ritter and Bozzelli)[38] (see Tables 23 and 24).

7.12. $\cdot C_6H_4ClO$ (2,4-cyclohexadiene-6-chloro-1-one-2-yl radical)

No experimental data are available for this radical. It is calculated here for the first time. Only CHEM3D-MOPAC-2000 version of MOPAC could differentiate between this radical and the former one. The AM1 UHF calculation gave a transition state, not a radical. The thermodynamics of this radical was calculated using PM3 (see Tables 25 and 26).

We have estimated the enthalpy of formation to be 230 $\pm$125 kJ mol^{-1} (55$\pm$30 kcal/mol^{-1}) to comply with the MOPAC/Thergas difference found for the previous radical (see Sec. 7.11).

7.13. $C_6H_4Cl_2O$ (2,4-dichlorophenol)

The spectral IR molecular vibration values[26] were supplemented with MOPAC PM3 calculations.

The experimental enthalpy of formation approximation of

TABLE 10. Thermodynamic properties of $C_6H_2Cl_3O\cdot$ (2,4,6-trichlorophenoxy radical) (M_r=196.439)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	$C_p°$ (J·K^{-1}·mol^{-1})	$H°-H°(T_r)$ (J·mol^{-1})	$S°$ (J·K^{-1}·mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}·mol^{-1})	$H(T)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	log K_f
0	—	−26.1522	—	—	−58.8502	−25.9495	—
100	69.579	−21.3409	293.5545	506.9638	−54.0389	−30.3242	6.2818
200	109.244	−12.3178	354.5165	416.1056	−45.0158	−31.9694	−1.8381
298.15	140.784	0.0000	404.2073	404.2073	−32.6980	−32.6980	−4.6176
300	141.323	0.2609	405.0799	404.2100	−32.4370	−32.7068	−4.6529
400	167.509	15.7509	449.4610	410.0837	−16.9471	−32.9534	−6.0827
500	188.191	33.5785	489.1563	421.9993	0.8806	−32.8944	−6.9433
600	204.292	53.2363	524.9520	436.2249	20.5383	−32.6581	−7.5141
700	216.879	74.3201	557.4280	451.2564	41.6221	−32.2822	−7.9181
800	226.836	96.5247	587.0633	466.4074	63.8267	−31.7768	−8.2172
900	234.820	119.6217	614.2585	481.3454	86.9238	−31.1444	−8.4456
1000	241.305	143.4389	639.3464	495.9075	110.7410	−30.4123	−8.6244
1100	246.631	167.8442	662.6031	510.0174	135.1463	−29.5920	−8.7669
1200	251.048	192.7349	684.2580	523.6456	160.0369	−28.7033	−8.8823
1300	254.744	218.0298	704.5028	536.7875	185.3318	−27.7694	−8.9772
1400	257.860	243.6643	723.4986	549.4526	210.9664	−26.8209	−9.0552
1500	260.508	269.5863	741.3818	561.6576	236.8883	−25.8530	−9.1211
1600	262.773	295.7532	758.2688	573.4230	263.0552	−24.8975	−9.1764
1700	264.721	322.1303	774.2592	584.7708	289.4323	−23.9660	−9.2233
1800	266.409	348.6888	789.4391	595.7232	315.9908	−23.0686	−9.2635
1900	267.877	375.4047	803.8833	606.3019	342.7068	−22.2136	−9.2981
2000	269.162	402.2581	817.6570	616.5280	369.5601	−21.4087	−9.3278
2100	270.292	429.2320	830.8174	626.4212	396.5340	−20.6623	−9.3541
2200	271.290	456.3122	843.4149	636.0003	423.6142	−19.9917	−9.3770
2300	272.176	483.4864	855.4942	645.2828	450.7884	−19.3910	−9.3974
2400	272.965	510.7441	867.0949	654.2848	478.0462	−18.8732	−9.4157
2500	273.670	538.0765	878.2524	663.0218	505.3786	−18.4568	−9.4317
2600	274.303	565.4757	888.9985	671.5079	532.7778	−18.1267	−9.4463
2700	274.873	592.9350	899.3617	679.7561	560.2370	−17.9054	−9.4599
2800	275.388	620.4485	909.3676	687.7789	587.7505	−17.7934	−9.4724
2900	275.854	648.0109	919.0396	695.5875	615.3130	−17.7940	−9.4836
3000	276.278	675.6179	928.3988	703.1928	642.9200	−17.9251	−9.4941
3100	276.665	703.2654	937.4643	710.6045	670.5674	−18.1622	−9.5045
3200	277.018	730.9498	946.2537	717.8319	698.2518	−18.5318	−9.5142
3300	277.341	758.6679	954.7830	724.8836	725.9700	−19.0255	−9.5233
3400	277.638	786.4171	963.0669	731.7678	753.7191	−19.6434	−9.5322
3500	277.911	814.1947	971.1189	738.4919	781.4968	−20.3944	−9.5412
3600	278.163	841.9986	978.9515	745.0630	809.3006	−21.2590	−9.5497
3700	278.396	869.8267	986.5761	751.4878	837.1287	−22.2510	−9.5584
3800	278.611	897.6771	994.0033	757.7725	864.9792	−23.3594	−9.5667
3900	278.811	925.5483	1001.2430	763.9229	892.8504	−24.5783	−9.5752
4000	278.996	953.4388	1008.3042	769.9445	920.7408	−25.9179	−9.5835
4100	279.169	981.3472	1015.1955	775.8426	948.6492	−27.3465	−9.5922
4200	279.330	1009.2722	1021.9248	781.6219	976.5743	−28.8804	−9.6008
4300	279.480	1037.2128	1028.4993	787.2871	1004.5149	−30.5139	−9.6091
4400	279.621	1065.1680	1034.9261	792.8425	1032.4700	−32.2503	−9.6175
4500	279.752	1093.1367	1041.2115	798.2922	1060.4388	−34.0511	−9.6263
4600	279.876	1121.1182	1047.3615	803.6401	1088.4202	−35.9236	−9.6351
4700	279.992	1149.1116	1053.3818	808.8900	1116.4137	−37.8586	−9.6440
4800	280.101	1177.1163	1059.2777	814.0452	1144.4183	−39.8520	−9.6532
4900	280.203	1205.1315	1065.0543	819.1091	1172.4336	−41.8993	−9.6625
5000	280.300	1233.1567	1070.7161	824.0848	1200.4587	−44.0552	−9.6713
5100	280.391	1261.1913	1076.2677	828.9753	1228.4933	−46.1845	−9.6810
5200	280.477	1289.2347	1081.7132	833.7834	1256.5367	−48.3958	−9.6903
5300	280.558	1317.2864	1087.0565	838.5119	1284.5884	−50.6438	−9.6996
5400	280.635	1345.3461	1092.3015	843.1633	1312.6481	−52.9282	−9.7092
5500	280.708	1373.4132	1097.4515	847.7400	1340.7153	−55.2433	−9.7187
5600	280.777	1401.4875	1102.5101	852.2445	1368.7895	−57.5864	−9.7282
5700	280.842	1429.5685	1107.4803	856.6788	1396.8705	−59.9548	−9.7379
5800	280.905	1457.6559	1112.3652	861.0452	1424.9579	−62.3467	−9.7475
5900	280.964	1485.7493	1117.1676	865.3457	1453.0513	−64.7588	−9.7572
6000	281.020	1513.8485	1121.8903	869.5822	1481.1506	−67.1869	−9.7669

TABLE 11. Molecular properties of $C_6H_2Cl_3O$ (2,4,6-trichlorophenol-3-yl radical). Values listed with bold characters were chosen for thermodynamic calculations—$\sigma = \mathbf{1}$ and statistical weight = **2**

	Enthalpy of formation $\Delta_f H°(298.15\ K)$ / kcal mol^{-1}	Zero point energy ZPE / kcal mol^{-1}
Our estimate	**16.86±5**	
NIST 94[35]	16.3	
THERM[38]	21.87	
THERGAS[37]	Failed	
PM3	18.69	41.706
PM3 UHF	10.94	40.435
AM1	22.88	42.528
AM1 UHF	14.58	41.350

Moments of inertia of the molecule / g cm$^2\times10^{-39}$

MOPAC method	I_a	I_b	I_c
PM3	**97.916 68**	**114.720 54**	**212.6372**
PM3 UHF	97.916 68	114.720 54	212.6372
AM1	99.476 24	115.717 27	215.1932
AM1 UHF	99.684 87	115.994 76	215.6795

Reduced moment of inertia[34] $I_r = \mathbf{0.1424}$ g cm$^2\times10^{-39}$; $\boldsymbol{\sigma}_{rot} = \mathbf{2}$; $V(2) = \mathbf{1116.8}$ cm^{-1}.

Molecular vibrations / cm^{-1}

PM3	100.7	**142**	**168**	**191**	**223**	**292**
	300	**364**	**379**	**425**	**456**	**545**
	568	**678**	**746**	**792**	**821**	**898**
	1008	**1101**	**1212**	**1282**	**1409**	**1438**
	1525	**1613**	**1728**	**1864**	**3065**	**3854**
PM3 UHF	81.1	127.5	168.7	170	191	274
	299	326	360	374	418	490
	561	568	705	733	775	878
	893	1091	1183	1321	1373	1484
	1493	1594	1656	1781	3062	3854
AM1	93.63	151	182	206	221	294
	315	400	418	442	465	546
	601	718	766	863	904	978
	985	1211	1296	1337	1479	1499
	1548	1675	1716	1841	3182	3406
AM1 UHF	79.5	133	183	187	205	262
	315	351	395	438	458	517
	580	594	682	852	896	900
	960	1197	1289	1348	1454	1495
	1499	1637	1656	1756	3178	3409

Da Silva *et al.*[43] quoted in the NIST WebBook 2000[7] was adopted (see Tables 27 and 28).

7.14. C_6H_5ClO (o-chlorophenol)

Only the IR spectra of this compound is available. This compound was calculated by Shaub[36] using Benson's group additivity method.[32] The MOPAC method was used to calculate the molecular vibrations and the moments of inertia. The PM3 UHF calculation failed. The NIST 94 estimate was preferred over the other because it is the average between Thergas and Shaub's and because it is close to the MOPAC calculations which are quite consistent. The thermodynamic properties were calculated using the IR spectra with PM3 additions as marked in Table 29 (see also Table 30).

7.15. $\cdot C_6H_5O$ (2,4-cyclohexadiene-1-one-2-yl radical)

This radical is an unchlorinated species connected with the kinetics of chlorodibenzodioxins and chlorodibenzofurans. It does not appear in any thermodynamic compendium. It was calculated using the MOPAC PM3 method.

The enthalpy of formation was estimated using Thergas (see Tables 31 and 32).[37]

7.16. $C_{12}H_4OCl_4$ (2,3,6,7-tetrachlorodibenzofuran)

This specie was published by Dorofeeva *et al.*[39] Dorofeeva's calculated vibrations and moments of inertia using the DFT B3LYP method were obtained as a private communication.[48] $\Delta_f H°(298.15\ K) = -50. \pm 10$ kJ mol^{-1}. For comparison purposes we have calculated the PM3 data

TABLE 12. Thermodynamic properties of $C_6HCl_3OH\cdot$ (2,4,6-trichlorophenol-3-yl radical) (M_r=196.439)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	C_p° ($J\cdot K^{-1}\cdot mol^{-1}$)	$H°-H°(T_r)$ ($J\cdot mol^{-1}$)	$S°$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$-[G°-H°(T_r)]/T$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$H(T)$ ($kJ\cdot mol^{-1}$)	$\Delta_f H°$ ($kJ\cdot mol^{-1}$)	log K_f
0	—	−25.296	—	—	45.267	78.168	—
100	63.752	−21.018	288.975	499.153	49.545	73.260	−48.0631
200	108.336	−12.295	347.653	409.129	58.268	71.314	−29.1710
298.15	140.745	0.000	397.240	397.240	70.563	70.563	−23.0721
300	141.278	0.261	398.112	397.243	70.824	70.554	−22.9958
400	166.659	15.711	442.385	403.107	86.274	70.268	−19.9314
500	186.358	33.404	481.783	414.976	103.967	70.192	−18.0976
600	201.627	52.835	517.169	429.110	123.398	70.202	−16.8753
700	213.536	73.617	549.181	444.013	144.181	70.276	−16.0018
800	222.949	95.459	578.333	459.009	166.023	70.419	−15.3459
900	230.505	118.145	605.044	473.772	188.709	70.640	−14.8343
1000	236.663	141.514	629.660	488.146	212.077	70.923	−14.4236
1100	241.751	165.442	652.462	502.060	236.006	71.267	−14.0860
1200	246.002	189.836	673.685	515.488	260.399	71.658	−13.8032
1300	249.589	214.621	693.521	528.429	285.184	72.082	−13.5629
1400	252.642	239.736	712.133	540.892	310.299	72.511	−13.3551
1500	255.258	265.135	729.655	552.898	335.698	72.955	−13.1745
1600	257.516	290.776	746.202	564.467	361.339	73.385	−13.0154
1700	259.475	316.628	761.874	575.623	387.191	73.791	−12.8741
1800	261.185	342.663	776.755	586.387	413.226	74.165	−12.7478
1900	262.684	368.858	790.918	596.782	439.421	74.499	−12.6342
2000	264.004	395.193	804.426	606.829	465.757	74.786	−12.5314
2100	265.173	421.653	817.335	616.548	492.217	75.018	−12.4384
2200	266.211	448.224	829.696	625.958	518.787	75.179	−12.3534
2300	267.136	474.892	841.550	635.075	545.455	75.273	−12.2758
2400	267.965	501.648	852.937	643.917	572.211	75.289	−12.2048
2500	268.709	528.482	863.891	652.498	599.045	75.207	−12.1390
2600	269.379	555.387	874.443	660.833	625.950	75.043	−12.0786
2700	269.985	582.356	884.622	668.934	652.919	74.774	−12.0230
2800	270.534	609.382	894.450	676.814	679.945	74.399	−11.9716
2900	271.034	636.461	903.953	684.483	707.024	73.914	−11.9236
3000	271.489	663.587	913.149	691.953	734.151	73.302	−11.8792
3100	271.905	690.757	922.058	699.233	761.320	72.588	−11.8385
3200	272.285	717.967	930.696	706.332	788.530	71.743	−11.8006
3300	272.635	745.213	939.081	713.258	815.777	70.778	−11.7652
3400	272.956	772.493	947.224	720.021	843.056	69.690	−11.7324
3500	273.253	799.804	955.141	726.626	870.367	68.472	−11.7023
3600	273.527	827.143	962.843	733.081	897.706	67.143	−11.6740
3700	273.780	854.508	970.341	739.392	925.072	65.688	−11.6481
3800	274.015	881.898	977.645	745.566	952.462	64.119	−11.6238
3900	274.233	909.311	984.765	751.609	979.874	62.441	−11.6016
4000	274.436	936.745	991.711	757.525	1007.308	60.645	−11.5808
4100	274.625	964.198	998.490	763.320	1034.761	58.761	−11.5620
4200	274.802	991.669	1005.110	768.998	1062.232	56.773	−11.5446
4300	274.967	1019.158	1011.578	774.565	1089.721	54.687	−11.5282
4400	275.121	1046.662	1017.901	780.023	1117.225	52.500	−11.5131
4500	275.266	1074.182	1024.086	785.379	1144.745	50.250	−11.4997
4600	275.402	1101.715	1030.137	790.634	1172.278	47.929	−11.4872
4700	275.530	1129.262	1036.061	795.793	1199.825	45.547	−11.4759
4800	275.650	1156.821	1041.864	800.859	1227.384	43.108	−11.4659
4900	275.763	1184.392	1047.548	805.836	1254.955	40.616	−11.4567
5000	275.869	1211.973	1053.121	810.726	1282.536	38.017	−11.4480
5100	275.970	1239.565	1058.585	815.533	1310.128	35.445	−11.4409
5200	276.065	1267.167	1063.944	820.258	1337.730	32.792	−11.4342
5300	276.155	1294.778	1069.204	824.906	1365.341	30.103	−11.4282
5400	276.240	1322.398	1074.366	829.478	1392.961	27.378	−11.4230
5500	276.321	1350.026	1079.436	833.977	1420.589	24.624	−11.4185
5600	276.398	1377.662	1084.416	838.405	1448.225	21.843	−11.4145
5700	276.470	1405.305	1089.308	842.764	1475.869	19.037	−11.4112
5800	276.539	1432.956	1094.117	847.056	1503.519	16.208	−11.4084
5900	276.605	1460.613	1098.845	851.284	1531.176	13.359	−11.4061
6000	276.668	1488.277	1103.495	855.448	1558.840	10.495	−11.4043

TABLE 13. Molecular properties of $C_6H_2Cl_3O_3$· (2,4,6-trichlorobicyclo-2,5-hexadiene-1,4-peroxy-1-phenoxy radical). Values listed with bold characters were chosen for thermodynamic calculations

	Enthalpy of formation $\Delta_f H°(298.15\ K)$ / kcal mol^{-1}	Zero point energy ZPE / kcal mol^{-1}
Our estimate	**30.7**	
PM3	36.999	45.234
PM3 UHF	24.004	44.982
AM1	61.691	48.183
AM1 UHF	47.109	48.012

Moments of inertia of the molecule / g cm^2×10^{-39}

Method	I_a	I_b	I_c
Gaussian 98/HF	110.4929	142.0306	207.6226
PM3	**107.3237**	**144.5280**	**201.7532**
PM3 UHF	105.5388	145.7740	199.9214
AM1	107.1465	144.0010	201.1460
AM1 UHF	106.3286	144.7438	200.5527

Molecular vibrations / cm^{-1}

Gaussian 98	79.1(71.2)	135(121.5)	174(156.6)	176(158.4)	225(203)	244(220)
HF/6-31G(d)	251(226)	341(307)	344(310)	392(353)	410(369)	425(383)
(scaled 0.9)	466(419)	509(458)	529(476)	541(487)	592(533)	662(596)
	749(674)	761(685)	786(707)	809(728)	843(759)	858(772)
	917(825)	918(826)	995(896)	1072(965)	1158(1042)	1194(1075)
	1224(1102)	1280(1152)	1663(1497)	1685(1517)	3256(2930)	3258(2932)
PM3	**92.3**	**146**	**165**	**171**	**215**	**217**
	253	**341**	**344**	**366**	**394**	**411**
	506	**547**	**555**	**571**	**693**	**741**
	812	**833**	**889**	**928**	**952**	**975**
	1092	**1115**	**1144**	**1191**	**1203**	**1268**
	1270	**1354**	**1783**	**1849**	**3120**	**3123**
PM3 UHF	86.56	144	165	172	219	232
	264	340	342	366	401	438
	483	548	557	573	675	712
	799	827	885	904	930	970
	1064	1123	1184	1189	1195	1249
	1275	1463	1708	1729	3115	3117
AM1	95.2	130	177	186	192	250
	260	379	394	443	449	463
	542	582	598	634	783	840
	923	935	978	1001	1031	1139
	1145	1165	1231	1254	1301	1341
	1388	1438	1775	1810	3228	3232
AM1 UHF	90.2	142	177	191	208	247
	266	375	392	448	463	463
	521	579	608	632	754	832
	904	930	936	998	1028	1089
	1151	1159	1266	1270	1297	1353
	1371	1590	1685	1703	3220	3223

for this molecule. PM3 UHF calculations failed and AM1 resulted in a transition state (see Tables 33 and 34).

7.17. $C_{12}H_4OCl_4$ (2,4,6,8-tetrachlorodibenzofuran)

This specie was published by Dorofeeva *et al.*[39] $\Delta_f H°(298.15\ K) = -58 \pm 10\ kJ\ mol^{-1}$. Dorofeeva's calculated vibrations and moments of inertia by the DFT B3LYP method were obtained as private communication.[48] The PM3 data are presented for comparison purposes. The PM3 UHF calculations show transition state (see Tables 35 and 36).

7.18. $C_{12}H_4O_2Cl_4$ (2,3,7,8-tetrachlorodibenzo-*p*-dioxin)

This species was published by Dorofeeva, Iorish and Moiseeva (1999).[39] $\Delta_f H°(298.15\ K) = -164.0 \pm 15.\ kJ\ mol^{-1}$. Recently, Mhin *et al.*,[44] published vibrations of 76 chloro dibenzo-*p*-dioxin congeners using the GAUSSIAN 98 B3LYP/6-31G** method and basis set. These vibrations served us to calculate the thermodynamic properties of this species. The moments of inertia were taken from the PM3 calculation. A second calculation of PM3 results is given for comparison purposes (see Tables 37 and 38).

TABLE 14. Thermodynamic properties of $C_6H_2Cl_3O_3$· (2,4,6-trichlorobicyclo-2,5-hexadiene-1,4-peroxy-1-phenoxy radical) (M_r= 228.438)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	C_p° ($J\cdot K^{-1}\cdot mol^{-1}$)	$H°-H°(T_r)$ ($J\cdot mol^{-1}$)	$S°$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$-[G°-H°(T_r)]/T$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$H(T)$ ($kJ\cdot mol^{-1}$)	$\Delta_f H°$ ($kJ\cdot mol^{-1}$)	log K_f
0	—	−29.185	—	—	99.264	140.845	—
100	74.453	−24.377	300.354	544.122	104.072	133.566	−88.0208
200	124.852	−14.312	368.113	439.671	114.137	130.052	−53.5490
298.15	165.590	0.000	425.792	425.792	128.449	128.449	−42.4374
300	166.288	0.307	426.819	425.796	128.756	128.431	−42.2985
400	199.881	18.684	479.453	432.744	147.132	128.100	−36.7185
500	225.670	40.021	526.960	446.917	168.470	128.610	−33.3684
600	245.122	63.606	569.907	463.896	192.055	129.613	−31.1212
700	259.912	88.891	608.853	481.867	217.340	130.935	−29.5018
800	271.357	115.478	644.338	499.991	243.927	132.484	−28.2739
900	280.381	143.082	676.841	517.861	271.531	134.218	−27.3068
1000	287.619	171.495	706.770	535.275	299.943	136.082	−26.5227
1100	293.508	200.561	734.469	552.141	329.010	138.052	−25.8720
1200	298.360	230.162	760.222	568.420	358.611	140.101	−25.3218
1300	302.399	260.206	784.268	584.109	388.655	142.199	−24.8495
1400	305.792	290.620	806.806	599.220	419.069	144.312	−24.4381
1500	308.667	321.347	828.004	613.772	449.796	146.442	−24.0770
1600	311.121	352.340	848.005	627.793	480.788	148.553	−23.7561
1700	313.229	383.560	866.932	641.308	512.008	150.633	−23.4689
1800	315.052	414.976	884.888	654.346	543.425	152.669	−23.2100
1900	316.637	446.562	901.965	666.933	575.011	154.651	−22.9753
2000	318.023	478.297	918.243	679.095	606.746	156.571	−22.7611
2100	319.242	510.161	933.789	690.855	638.610	158.418	−22.5655
2200	320.317	542.140	948.666	702.238	670.589	160.174	−22.3853
2300	321.271	574.221	962.926	713.265	702.669	161.845	−22.2191
2400	322.120	606.391	976.617	723.955	734.840	163.417	−22.0655
2500	322.879	638.642	989.783	734.326	767.090	164.870	−21.9223
2600	323.560	670.964	1002.460	744.397	799.413	166.220	−21.7893
2700	324.174	703.351	1014.683	754.182	831.800	167.443	−21.6652
2800	324.727	735.797	1026.482	763.698	864.246	168.540	−21.5494
2900	325.229	768.295	1037.886	772.957	896.744	169.507	−21.4404
3000	325.685	800.841	1048.920	781.973	929.290	170.327	−21.3382
3100	326.101	833.431	1059.606	790.757	961.880	171.024	−21.2426
3200	326.481	866.060	1069.965	799.321	994.509	171.571	−21.1524
3300	326.828	898.726	1080.017	807.676	1027.175	171.978	−21.0673
3400	327.147	931.425	1089.779	815.830	1059.874	172.244	−20.9871
3500	327.441	964.155	1099.266	823.793	1092.603	172.363	−20.9117
3600	327.712	996.912	1108.494	831.574	1125.361	172.352	−20.8401
3700	327.962	1029.696	1117.477	839.180	1158.145	172.200	−20.7727
3800	328.194	1062.504	1126.226	846.620	1190.953	171.917	−20.7085
3900	328.408	1095.334	1134.754	853.899	1223.783	171.509	−20.6481
4000	328.608	1128.185	1143.071	861.025	1256.634	170.966	−20.5906
4100	328.794	1161.056	1151.187	868.003	1289.504	170.321	−20.5365
4200	328.967	1193.944	1159.113	874.840	1322.392	169.558	−20.4850
4300	329.128	1226.848	1166.855	881.542	1355.297	168.683	−20.4359
4400	329.279	1259.769	1174.424	888.112	1388.218	167.693	−20.3892
4500	329.421	1292.704	1181.825	894.557	1421.153	166.625	−20.3451
4600	329.553	1325.653	1189.067	900.881	1454.102	165.474	−20.3031
4700	329.678	1358.614	1196.156	907.089	1487.063	164.249	−20.2633
4800	329.795	1391.588	1203.098	913.183	1520.037	162.954	−20.2257
4900	329.905	1424.573	1209.899	919.170	1553.022	161.593	−20.1898
5000	330.009	1457.569	1216.565	925.051	1586.018	160.115	−20.1552
5100	330.107	1490.575	1223.101	930.831	1619.024	158.651	−20.1230
5200	330.199	1523.590	1229.512	936.514	1652.039	157.095	−20.0918
5300	330.287	1556.614	1235.802	942.102	1685.063	155.494	−20.0622
5400	330.369	1589.647	1241.977	947.598	1718.096	153.844	−20.0341
5500	330.448	1622.688	1248.040	953.006	1751.137	152.155	−20.0072
5600	330.522	1655.737	1253.995	958.327	1784.185	150.430	−19.9815
5700	330.592	1688.792	1259.845	963.566	1817.241	148.671	−19.9570
5800	330.659	1721.855	1265.595	968.724	1850.304	146.880	−19.9337
5900	330.723	1754.924	1271.248	973.804	1883.373	145.061	−19.9113
6000	330.783	1787.999	1276.807	978.808	1916.448	143.219	−19.8901

TABLE 15. Molecular properties of $C_6H_2Cl_3O_3$· (2,4,6-trichlorobicyclo-2-hexene-1-one-4,6-peroxy-5-yl radical). Values listed with bold characters were chosen for thermodynamic calculations—$\sigma = \mathbf{1}$ and statistical weight = **2**

	Enthalpy of formation $\Delta_f H°(298.15\ \mathrm{K})$ / kcal mol^{-1}	Zero point energy ZPE / kcal mol^{-1}
Our estimate	**−2.08**	
PM3	−1.779	44.956
PM3 UHF	−6.059	44.780
AM1	30.34	47.895
AM1 UHF	25.94	47.679

Moments of inertia of the molecule / g cm^2 × 10^{-39}

Method	I_a	I_b	I_c
Gaussian 98 HF	116.3316	128.6100	220.1830
PM3	**119.6179**	**130.9715**	**223.8863**
PM3 UHF	119.6179	130.9715	223.8863
AM1	118.0182	129.7836	222.1650
AM1 UHF	117.8944	130.0073	222.1323

Molecular vibrations / cm^{-1}

Gaussian 98	77.6(69.8)	152(137)	175.6(158)	191(172)	220(198)	267(240)
HF/6-31G(d)	315(283)	343(309)	373(336)	405(364)	431(388)	444(400)
(scaled 0.9)	485(437)	559(503)	583(525)	688(619)	781(703)	829(746)
	869(782)	893(804)	939(845)	1012(911)	1042(938)	1066(959)
	1134(1021)	1195(1076)	1209(1088)	1246(1121)	1283(1155)	1308(1177)
	1427(1284)	1461(1315)	1828(1645)	2065(1856)	3419(3077)	3432(3089)
PM3	**63.1**	**132**	**149**	**171**	**205**	**231**
	279	**303**	**325**	**356**	**385**	**403**
	435	**492**	**502**	**600**	**654**	**751**
	769	**802**	**827**	**890**	**929**	**971**
	1054	**1099**	**1176**	**1204**	**1227**	**1300**
	1302	**1360**	**1821**	**2002**	**3073**	**3188**
PM3 UHF	63	131	150	171	207	234
	279	302	330	355	388	405
	433	487	500	599	654	750
	767	800	823	887	924	967
	1047	1095	1167	1197	1219	1291
	1296	1343	1794	1996	3072	3184
AM1	55.8	136	162	185	213	238
	309	323	353	412	422	440
	471	524	566	686	743	813
	866	917	956	980	1023	1109
	1147	1167	1209	1283	1308	1356
	1380	1397	1817	2085	3183	3291
AM1 UHF	54.4	136	163	184	213	237
	308	322	357	412	419	439
	466	519	556	682	728	810
	864	914	953	974	1019	1096
	1140	1164	1192	1269	1310	1345
	1379	1396	1794	2084	3184	3285

7.19. $C_{12}H_4O_2Cl_4$ (1,3,6,8-tetrachlorodibenzo-*p*-dioxin)

This species was published by Dorofeeva *et al.*[39] $\Delta_f H°(298.15\ \mathrm{K}) = -173.0 \pm 15.\ \mathrm{kJ\,mol^{-1}}$. Asatryan *et al.*[45] have calculated $\Delta_f H°(298.15\ \mathrm{K}) = -131.92\ \mathrm{kJ\,mol^{-1}}$ for this specie, using PM3 methods. Recently, Mhin *et al.*[44] published the molecular vibrations of 76 chlorodibenzo-*p*-dioxin congeners using the GAUSSIAN 98 B3LYP/6-31G** method and basis set. Dorofeeva has also sent us her unpublished results[48] which are closer to the PM3 values. Mhin's vibrations[44] served us to calculate the thermodynamic properties of this specie. The moments of inertia were taken from the PM3 calculation (see Tables 39 and 40).

7.20. $C_{12}H_4Cl_4O_3$ (1,3,6,8-tetrachlorodibenzo-*p*-dioxin-2-ol)

This compound a tetrachloro *p*-dibenzo dioxine alcohol was calculated using MOPAC, and its enthalpy of formation

TABLE 16. Thermodynamic properties of $C_6H_2Cl_3O_3$· (2,4,6-trichlorobicyclo-2-hexene-1-one-5-yl-4,6-peroxy radical) (M_r=228.438)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	C_p° (J·K^{-1}·mol^{-1})	$H°-H°(T_r)$ (J·mol^{-1})	$S°$ (J·K^{-1}·mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}·mol^{-1})	$H(T)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	log K_f
0	—	−30.072	—	—	−38.774	2.807	—
100	76.914	−25.066	305.039	555.699	−33.769	−4.275	−15.7773
200	128.639	−14.674	375.011	448.378	−23.376	−7.462	−17.2748
298.15	168.984	0.000	434.167	434.167	−8.703	−8.703	−17.9722
300	169.666	0.313	435.215	434.171	−8.389	−8.714	−17.9814
400	202.272	18.979	488.688	441.240	10.276	−8.756	−18.3650
500	227.183	40.510	536.629	455.610	31.807	−8.053	−18.5866
600	246.012	64.213	579.793	472.771	55.510	−6.931	−18.7179
700	260.397	89.565	618.844	490.895	80.862	−5.543	−18.7961
800	271.588	116.186	654.376	509.143	107.484	−3.959	−18.8410
900	280.456	143.805	686.896	527.113	135.102	−2.211	−18.8637
1000	287.599	172.220	716.828	544.607	163.518	−0.344	−18.8714
1100	293.433	201.281	744.522	561.538	192.579	1.621	−18.8685
1200	298.252	230.873	770.267	577.872	222.170	3.661	−18.8582
1300	302.274	260.905	794.303	593.607	252.203	5.747	−18.8428
1400	305.660	291.307	816.831	608.755	282.604	7.847	−18.8230
1500	308.533	322.020	838.020	623.340	313.318	9.964	−18.8013
1600	310.988	352.999	858.013	637.388	344.297	12.061	−18.7775
1700	313.100	384.206	876.932	650.928	375.504	14.128	−18.7524
1800	314.928	415.610	894.881	663.986	406.907	16.152	−18.7265
1900	316.519	447.184	911.952	676.592	438.482	18.122	−18.7004
2000	317.911	478.907	928.223	688.770	470.205	20.030	−18.6738
2100	319.135	510.761	943.764	700.545	502.058	21.866	−18.6480
2200	320.216	542.730	958.636	711.941	534.027	23.612	−18.6222
2300	321.176	574.800	972.892	722.979	566.097	25.273	−18.5970
2400	322.030	606.961	986.579	733.679	598.258	26.836	−18.5726
2500	322.794	639.203	999.741	744.060	630.500	28.280	−18.5484
2600	323.480	671.517	1012.415	754.139	662.815	29.622	−18.5251
2700	324.098	703.897	1024.635	763.932	695.194	30.837	−18.5027
2800	324.656	736.335	1036.432	773.455	727.632	31.926	−18.4812
2900	325.161	768.826	1047.833	782.721	760.124	32.887	−18.4601
3000	325.621	801.366	1058.865	791.743	792.663	33.700	−18.4399
3100	326.040	833.949	1069.549	800.533	825.246	34.390	−18.4211
3200	326.423	866.573	1079.906	809.102	857.870	34.932	−18.4028
3300	326.773	899.233	1089.956	817.461	890.530	35.333	−18.3853
3400	327.095	931.926	1099.716	825.620	923.223	35.594	−18.3687
3500	327.391	964.651	1109.202	833.588	955.948	35.708	−18.3532
3600	327.665	997.404	1118.429	841.372	988.701	35.692	−18.3383
3700	327.917	1030.183	1127.410	848.982	1021.480	35.535	−18.3245
3800	328.151	1062.986	1136.158	856.425	1054.284	35.248	−18.3111
3900	328.367	1095.813	1144.685	863.707	1087.110	34.835	−18.2989
4000	328.569	1128.659	1153.001	870.836	1119.957	34.289	−18.2871
4100	328.756	1161.526	1161.117	877.818	1152.823	33.640	−18.2766
4200	328.931	1194.410	1169.041	884.658	1185.707	32.873	−18.2666
4300	329.094	1227.311	1176.783	891.361	1218.609	31.994	−18.2569
4400	329.246	1260.229	1184.350	897.935	1251.526	31.001	−18.2480
4500	329.389	1293.160	1191.751	904.382	1284.458	29.930	−18.2400
4600	329.523	1326.106	1198.992	910.708	1317.403	28.775	−18.2325
4700	329.649	1359.065	1206.080	916.917	1350.362	27.547	−18.2257
4800	329.767	1392.036	1213.022	923.014	1383.333	26.250	−18.2197
4900	329.878	1425.018	1219.822	929.002	1416.315	24.887	−18.2142
5000	329.983	1458.011	1226.488	934.886	1449.308	23.405	−18.2087
5100	330.081	1491.014	1233.023	940.668	1482.311	21.939	−18.2045
5200	330.175	1524.027	1239.434	946.352	1515.324	20.381	−18.2003
5300	330.263	1557.049	1245.724	951.941	1548.346	18.777	−18.1966
5400	330.347	1590.079	1251.898	957.439	1581.377	17.125	−18.1934
5500	330.426	1623.118	1257.960	962.848	1614.415	15.434	−18.1905
5600	330.501	1656.164	1263.915	968.171	1647.462	13.707	−18.1880
5700	330.572	1689.218	1269.765	973.411	1680.515	11.945	−18.1859
5800	330.639	1722.279	1275.515	978.570	1713.576	10.152	−18.1842
5900	330.704	1755.346	1281.168	983.651	1746.643	8.331	−18.1827
6000	330.765	1788.419	1286.726	988.656	1779.717	6.487	−18.1816

TABLE 17. Molecular properties of $C_6H_3Cl_3O$ (2,4,6-trichlorophenol). Values listed with bold characters were chosen for thermodynamic calculations—σ = **2** and statistical weight = **1**

	Enthalpy of formation $\Delta_f H°(298.15\ K)$ / kcal mol^{-1}	Zero point energy ZPE/kcal mol^{-1}
Our estimate	**−41.5±9.0**	
Shaub[21]	−34.28	
PM3	−38.81	48.239
PM3 UHF	−39.03	47.890
AM1	−38.42	49.597
AM1 UHF	−38.92	49.224

Moments of inertia of the molecule / g cm^2×10^{-39}

MOPAC method	I_a	I_b	I_c
PM3	**99.821 24**	**115.787 54**	**215.609**
PM3 UHF	99.821 24	115.787 54	215.609
AM1	99.821 24	115.787 54	215.609
AM1 UHF	99.928 91	115.924 18	215.852

Reduced moment of inertia[34] I_r = **0.14239** g cm^2×10^{-39}; σ_{rot} = **2**; $V(2)$ = **1116.8** cm^{-1}.

Molecular vibrations / cm^{-1}

Ir[26]		**564**	**733**	**809**	**847**	**918**
	1067	**1076**	**1109**	**1168**	**1223**	**1261**
	1321	**1397**	**1468**	**1572**	**1713**	**1724**
	3095	**3569**	**3857**			
PM3	105.1	**148.8**	**184**	**194**	**204**	**307**
	357	**360**	**368**	**419**	**528**	**568**
	570	612	715	756	770	887
	947	961	1084	1164	1188	1271
	1384	1437	1538	1573	1746	1750
	3007	3012	3629			
PM3 UHF	102.3	146.4	184.2	194	194	307
	351	356	366	417	515	555
	566	611	711	735	765	877
	931	943	1080	1151	1163	1319
	1352	1438	1530	1561	1715	1717
	3006	3012	3629			
AM1	84.9	141.3	186.8	197	210	265
	322	366	405	439	464	542
	570	597	728	848	905	943
	950	976	1189	1241	1319	1351
	1459	1490	1584	1661	1753	1757
	3170	3175	3404			
AM1 UHF	80.4	138.1	172.4	198	210	266
	322	354	402	437	461	522
	550	595	699	843	901	922
	928	965	1186	1252	1295	1393
	1462	1477	1574	1645	1712	1722
	3169	3174	3404			

we estimated from the former molecule (see Sec. 7.19) using Dorofeeva's coefficients[39] and Bozzelli's increments[46] for the alcoholic group and the OH–Cl interaction (see Tables 41 and 42).

7.21. $C_{12}H_4Cl_5O_2$· (2,4-dichlorophenoxy-1′,3′,5′-trichlorophenyl-6-6′-ether radical–$Cl_2C_6H_2(O·)$–O–$C_6H_2Cl_3$) (PD·)

This radical appears in the literature as the PD· radical was calculated using the MOPAC package. The enthalpy of formation was estimated using the NIST 94[35] prediction and Dorofeeva's 1,3 Cl correction (see Tables 43 and 44).[39]

7.22. $C_{12}H_4Cl_6O_2$ (2,4,6-trichlorocyclohexa-3,5-diene-1-one-1′,3′,5′-trichlorophenyl-2-6′-ether) (PP)

This intermediate ether, which belongs to a group of chloro isomers known in the literature as PP, was calculated using the MOPAC PM3 method.

Its enthalpy of formation was very roughly estimated as the average between the PM3 and the PM3 UHF results. The AM1UHF calculation, failed (see Tables 45 and 46).

TABLE 18. Thermodynamic properties of $C_6H_3Cl_3O$ (2,4,6-trichlorophenol) (M_r=197.447)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	C_p° ($J\cdot K^{-1}\cdot mol^{-1}$)	$H°-H°(T_r)$ ($J\cdot mol^{-1}$)	$S°$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$-[G°-H°(T_r)]/T$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$H(T)$ ($kJ\cdot mol^{-1}$)	$\Delta_f H°$ ($kJ\cdot mol^{-1}$)	log K_f
0	—	−25.619	—	—	−199.255	−162.120	—
100	65.305	−21.254	284.705	497.249	−194.890	−168.441	75.3318
200	109.086	−12.438	344.070	406.259	−186.074	−171.640	30.9748
298.15	143.262	0.000	394.214	394.214	−173.636	−173.636	16.1385
300	143.846	0.266	395.102	394.217	−173.370	−173.667	15.9510
400	172.267	16.122	440.523	400.217	−157.514	−174.999	8.3633
500	194.764	34.521	481.484	412.443	−139.115	−175.831	3.7818
600	212.207	54.906	518.604	427.093	−118.730	−176.331	0.7161
700	225.774	76.833	552.377	442.615	−96.803	−176.582	−1.4785
800	236.499	99.967	583.252	458.293	−73.669	−176.624	−3.1260
900	245.147	124.064	611.624	473.775	−49.572	−176.479	−4.4070
1000	252.248	148.945	637.832	488.887	−24.691	−176.185	−5.4304
1100	258.169	174.474	662.160	503.547	0.838	−175.760	−6.2661
1200	263.164	200.548	684.844	517.720	26.912	−175.228	−6.9606
1300	267.420	227.082	706.080	531.402	53.446	−174.615	−7.5466
1400	271.075	254.012	726.036	544.599	80.376	−173.953	−8.0464
1500	274.232	281.281	744.848	557.327	107.645	−173.242	−8.4786
1600	276.977	308.844	762.636	569.608	135.208	−172.516	−8.8550
1700	279.374	336.665	779.501	581.463	163.029	−171.788	−9.1856
1800	281.478	364.709	795.531	592.914	191.073	−171.071	−9.4782
1900	283.332	392.952	810.800	603.983	219.316	−170.376	−9.7390
2000	284.973	421.369	825.376	614.691	247.733	−169.713	−9.9724
2100	286.430	449.940	839.316	625.058	276.304	−169.091	−10.1833
2200	287.729	478.649	852.671	635.103	305.013	−168.531	−10.3740
2300	288.891	507.482	865.487	644.843	333.846	−168.028	−10.5478
2400	289.934	536.424	877.805	654.295	362.788	−167.596	−10.7068
2500	290.874	565.465	889.660	663.474	391.829	−167.256	−10.8523
2600	291.722	594.595	901.085	672.394	420.959	−166.993	−10.9866
2700	292.490	623.807	912.109	681.070	450.171	−166.832	−11.1109
2800	293.187	653.091	922.759	689.512	479.455	−166.774	−11.2263
2900	293.822	682.442	933.059	697.734	508.806	−166.822	−11.3334
3000	294.402	711.854	943.030	705.745	538.218	−166.997	−11.4333
3100	294.932	741.321	952.692	713.556	567.685	−167.274	−11.5275
3200	295.418	770.839	962.063	721.176	597.203	−167.681	−11.6157
3300	295.865	800.403	971.161	728.614	626.767	−168.209	−11.6987
3400	296.276	830.010	979.999	735.879	656.374	−168.860	−11.7770
3500	296.656	859.657	988.593	742.977	686.021	−169.644	−11.8515
3600	297.007	889.341	996.955	749.916	715.705	−170.540	−11.9219
3700	297.332	919.058	1005.097	756.703	745.422	−171.565	−11.9891
3800	297.634	948.806	1013.031	763.345	775.170	−172.706	−12.0528
3900	297.914	978.584	1020.766	769.847	804.948	−173.959	−12.1140
4000	298.175	1008.389	1028.311	776.214	834.753	−175.334	−12.1723
4100	298.419	1038.218	1035.677	782.453	864.582	−176.800	−12.2287
4200	298.646	1068.072	1042.871	788.568	894.436	−178.374	−12.2826
4300	298.858	1097.947	1049.901	794.564	924.311	−180.050	−12.3342
4400	299.057	1127.843	1056.774	800.446	954.207	−181.831	−12.3838
4500	299.244	1157.758	1063.497	806.217	984.122	−183.681	−12.4321
4600	299.419	1187.691	1070.076	811.882	1014.055	−185.605	−12.4786
4700	299.584	1217.642	1076.517	817.444	1044.006	−187.595	−12.5237
4800	299.739	1247.608	1082.826	822.907	1073.972	−189.647	−12.5676
4900	299.885	1277.589	1089.008	828.275	1103.953	−191.756	−12.6101
5000	300.022	1307.584	1095.067	833.551	1133.948	−193.978	−12.6509
5100	300.152	1337.593	1101.010	838.737	1163.957	−196.177	−12.6913
5200	300.275	1367.615	1106.840	843.837	1193.979	−198.461	−12.7302
5300	300.391	1397.648	1112.560	848.853	1224.012	−200.786	−12.7680
5400	300.501	1427.693	1118.176	853.789	1254.057	−203.150	−12.8049
5500	300.606	1457.748	1123.691	858.646	1284.112	−205.548	−12.8408
5600	300.705	1487.814	1129.109	863.428	1314.178	−207.977	−12.8759
5700	300.799	1517.889	1134.432	868.136	1344.253	−210.434	−12.9101
5800	300.888	1547.973	1139.664	872.772	1374.337	−212.916	−12.9436
5900	300.973	1578.066	1144.808	877.339	1404.430	−215.421	−12.9762
6000	301.054	1608.168	1149.867	881.839	1434.532	−217.944	−13.0082

TABLE 19. Molecular properties of $C_6H_3Cl_3O_2$ (2-hydroxy-2,4,6-trichloro-3,5-cyclohexadiene-1-one). Values listed with bold characters were chosen for thermodynamic calculations—$\sigma=1$ and statistical weight = 1

	Enthalpy of formation $\Delta_f H°(298.15\ \text{K})$ / kcal mol^{-1}	Zero point energy ZPE / kcal mol^{-1}
Our estimate	**−63.0±6**	
THERM[38]	−57.2	
PM3	−64.48	50.544
PM3 UHF	−65.705	49.510
AM1	−60.516	52.416
AM1 UHF	−61.426	51.412

Moments of inertia of the molecule / g cm$^2\times10^{-39}$

MOPAC method	I_a	I_b	I_c
PM3	114.400 111	125.401 185	212.591 41
PM3 UHF	**110.199 475**	**128.255 082**	**204.094 373**
AM1	108.896 96	130.602 77	201.627 37
AM1 UHF	108.607 18	130.851 94	201.351 36

Reduced moment of inertia[34] $I_r=0.143\ 38$ g cm$^2\times10^{-39}$; $\sigma=2$; $V(2)=3.468$ kcal mol^{-1}.

Molecular vibrations / cm^{-1}

PM3	**22.1**	**90.1**	**140**	**175**	**187**	**243**
	278	**321**	**356**	**371**	**383**	**402**
	411	**485**	**541**	**606**	**671**	**740**
	802	**837**	**920**	**942**	**978**	**1090**
	1139	**1214**	**1249**	**1329**	**1387**	**1455**
	1828	**1838**	**1972**	**3042**	**3055**	**3873**
PM3 UHF	36.1	83.3	133	164	185	245
	287	331	350	362	367	395
	407	491	420	609	636	743
	781	835	886	909	961	1086
	1145	1208	1259	1350	1394	1409
	1472	1688	1954	3044	3052	3871
AM1	47.3	93.5	140	172	198	266
	311	347	377	393	410	437
	459	542	560	648	715	826
	867	928	955	961	1065	1187
	1227	1294	1362	1420	1444	1570
	1812	1835	2059	3159	3175	3412
AM1 UHF	47.8	89.6	135	171	197	266
	307	345	372	388	408	430
	452	525	548	645	703	808
	860	908	915	939	1063	1183
	1228	1294	1360	1419	1442	1478
	1573	1672	2040	3161	3180	3413

7.23. $C_{12}H_4Cl_6O_2$ or $C_6HCl_3OH-C_6HCl_3OH$ (2,4,6,2′,4′,6′-hexachloro-biphenyl-3,3′-diol)

No experimental data are available for this molecule. This intermediate stable species was calculated using the PM3 calculations. The three reduced moments of internal rotation were calculated using Wang's program. The PM3 UHF calculations failed. The thermodynamic properties were compared to a very rough approximation performed with NIST 94,[35] and THERM. These calculations gave very similar results, but THERM[37] was found to be not extrapolable by any method.

The $\Delta_f H°(298.15\ \text{K})=-321.92\pm33.5$ kJ mol^{-1} was estimated using THERM.[37] The enthalpy of formation of the 2,4,6,2′,4′,6′-hexachlorobiphenyl compound was reported by Dorofeeva *et al.*[47] as $\Delta_f H°(298.15\ \text{K})=43.60\pm15$ kJ mol^{-1} (10.42 ± 3.6 kcal mol^{-1}) (see Tables 47 and 48).

7.24. $C_{12}H_5Cl_3O_3$ (2,4,7-trichlorodibenzo-*p*-dioxin-9-ol)

There are no experimental data on this molecule. This molecule was calculated using the MOPAC PM3 method. The enthalpy of formation was estimated using Dorofeeva's[39] additivity increments and Bozzelli's increments[46] for the alcoholic group, and the Cl–OH interactions (see Tables 49 and 50).

TABLE 20. Thermodynamic properties of $C_6H_3Cl_3O_2$ (2-hydroxy-2,4,6-trichloro-3,5-cyclohexadiene-1-one) (M_r=213.447)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	C_p° ($J\cdot K^{-1}\cdot mol^{-1}$)	$H°-H°(T_r)$ ($J\cdot mol^{-1}$)	$S°$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$-[G°-H°(T_r)]/T$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$H(T)$ ($kJ\cdot mol^{-1}$)	$\Delta_f H°$ ($kJ\cdot mol^{-1}$)	log K_f
0	—	−28.939	—	—	−292.531	−251.056	—
100	72.184	−24.249	291.769	534.257	−287.841	−258.502	118.2164
200	125.011	−14.255	358.926	430.201	−277.847	−261.979	50.2911
298.15	163.778	0.000	416.401	416.401	−263.592	−263.592	27.6991
300	164.417	0.304	417.417	416.405	−263.288	−263.612	27.4144
400	194.712	18.327	469.058	423.240	−245.265	−264.263	15.9245
500	217.859	39.008	515.109	437.094	−224.584	−264.343	9.0208
600	235.611	61.719	556.468	453.603	−201.873	−264.097	4.4201
700	249.445	86.000	593.869	471.013	−177.592	−263.621	1.1383
800	260.446	111.514	627.923	488.530	−152.078	−262.951	−1.3179
900	269.359	138.020	659.131	505.776	−125.572	−262.101	−3.2226
1000	276.698	165.334	687.903	522.569	−98.258	−261.105	−4.7411
1100	282.816	193.319	714.571	538.827	−70.273	−259.981	−5.9783
1200	287.970	221.865	739.406	554.519	−41.727	−258.750	−7.0048
1300	292.348	250.887	762.634	569.644	−12.705	−257.443	−7.8693
1400	296.094	280.314	784.440	584.216	16.722	−256.092	−8.6059
1500	299.319	310.088	804.981	598.255	46.496	−254.697	−9.2416
1600	302.111	340.163	824.390	611.788	76.571	−253.294	−9.7945
1700	304.541	370.498	842.779	624.839	106.906	−251.898	−10.2796
1800	306.667	401.061	860.248	637.436	137.469	−250.523	−10.7084
1900	308.534	431.823	876.880	649.604	168.231	−249.180	−11.0900
2000	310.181	462.761	892.748	661.368	199.169	−247.879	−11.4313
2100	311.641	493.853	907.918	672.750	230.261	−246.631	−11.7390
2200	312.939	525.083	922.446	683.772	261.491	−245.457	−12.0171
2300	314.097	556.436	936.383	694.454	292.844	−244.351	−12.2700
2400	315.135	587.899	949.773	704.815	324.307	−243.328	−12.5009
2500	316.068	619.460	962.657	714.873	355.868	−242.409	−12.7121
2600	316.908	651.109	975.070	724.643	387.517	−241.579	−12.9065
2700	317.669	682.839	987.045	734.141	419.247	−240.862	−13.0861
2800	318.358	714.641	998.610	743.381	451.049	−240.260	−13.2525
2900	318.985	746.508	1009.793	752.376	482.916	−239.776	−13.4067
3000	319.556	778.436	1020.617	761.138	514.844	−239.429	−13.5503
3100	320.079	810.418	1031.103	769.678	546.826	−239.194	−13.6850
3200	320.557	842.450	1041.273	778.008	578.858	−239.101	−13.8109
3300	320.996	874.528	1051.144	786.136	610.936	−239.140	−13.9291
3400	321.400	906.648	1060.733	794.072	643.056	−239.310	−14.0404
3500	321.773	938.807	1070.055	801.824	675.215	−239.623	−14.1457
3600	322.117	971.002	1079.124	809.402	707.410	−240.058	−14.2449
3700	322.436	1003.230	1087.955	816.811	739.638	−240.629	−14.3393
3800	322.732	1035.488	1096.557	824.060	771.896	−241.327	−14.4287
3900	323.006	1067.775	1104.944	831.155	804.183	−242.144	−14.5140
4000	323.262	1100.089	1113.125	838.103	836.497	−243.092	−14.5950
4100	323.500	1132.427	1121.110	844.908	868.835	−244.139	−14.6729
4200	323.722	1164.788	1128.908	851.578	901.196	−245.301	−14.7472
4300	323.929	1197.171	1136.528	858.116	933.579	−246.572	−14.8180
4400	324.124	1229.574	1143.977	864.529	965.982	−247.957	−14.8860
4500	324.306	1261.995	1151.264	870.820	998.403	−249.416	−14.9517
4600	324.477	1294.434	1158.393	876.995	1030.842	−250.957	−15.0148
4700	324.637	1326.890	1165.373	883.056	1063.298	−252.571	−15.0756
4800	324.788	1359.362	1172.210	889.009	1095.770	−254.253	−15.1345
4900	324.931	1391.848	1178.908	894.857	1128.256	−255.999	−15.1913
5000	325.065	1424.347	1185.474	900.604	1160.755	−257.863	−15.2457
5100	325.192	1456.860	1191.912	906.253	1193.268	−259.711	−15.2992
5200	325.311	1489.386	1198.228	911.808	1225.794	−261.649	−15.3505
5300	325.425	1521.922	1204.426	917.271	1258.330	−263.633	−15.4003
5400	325.532	1554.470	1210.510	922.645	1290.878	−265.663	−15.4487
5500	325.633	1587.029	1216.484	927.933	1323.437	−267.732	−15.4956
5600	325.730	1619.597	1222.352	933.138	1356.005	−269.836	−15.5411
5700	325.821	1652.174	1228.118	938.263	1388.582	−271.973	−15.5855
5800	325.908	1684.761	1233.786	943.309	1421.169	−274.141	−15.6286
5900	325.991	1717.356	1239.357	948.280	1453.764	−276.335	−15.6705
6000	326.070	1749.959	1244.837	953.177	1486.367	−278.551	−15.7115

TABLE 21. Molecular properties of $C_6H_4ClO\cdot$ (o-chlorophenoxy radical). Values listed with bold characters were chosen for thermodynamic calculations—$\sigma = \mathbf{1}$ and statistical weight $= \mathbf{2}$

	Enthalpy of formation $\Delta_f H°(298.15\ \text{K})$ / kcal mol^{-1}	Zero point energy ZPE / kcal mol^{-1}
NIST 94[35]	**4.3±1**	
PM3	6.55	51.140
PM3 UHF	−3.61	53.320
AM1	9.23	53.320
AM1 UHF	−1.54	52.782

Moments of inertia of the molecule / g cm^2 × 10^{-39}

MOPAC method	I_a	I_b	I_c
PM3	**27.150 747**	**53.253 064**	**80.403 743**
PM3 UHF	27.256 96	53.622 64	80.8796
AM1	27.645 04	53.942 85	81.587 89
AM1 UHF	27.724 74	54.230 74	81.955 485

Molecular vibrations / cm^{-1}

PM3	**97.8**	**218**	**246**	**370**	**412**	**432**
	525	**552**	**689**	**697**	**778**	**868**
	871	**959**	**1001**	**1025**	**1090**	**1132**
	1151	**1178**	**1269**	**1392**	**1417**	**1603**
	1739	**1864**	**3046**	**3050**	**3067**	**3075**
PM3 UHF	89.0	208	243	374	390	410
	520	546	669	680	748	838
	860	906	948	1026	1093	1123
	1147	1187	1380	1391	1413	1567
	1609	1775	3049	3051	3065	3073
AM1	88.5	227	266	408	428	435
	547	588	708	756	812	906
	927	969	999	1124	1158	1200
	1225	1271	1322	1438	1467	1628
	1732	1957	3169	3173	3183	3192
AM1 UHF	87.5	216	264	407	409	419
	544	582	682	750	782	869
	920	925	954	1121	1158	1199
	1220	1277	1434	1449	1473	1585
	1627	1838	3173	3177	3185	3194

7.25. $C_{12}H_5Cl_4O_2\cdot$ (2,4-dichlorophenoxy-1′,3′-dichlorophenyl-6-6′-ether radical)

This radical is apparently more stable than its parent molecule $C_{12}H_6Cl_4O_2$. The AM1 UHF calculation failed. The enthalpy of formation was calculated from the NIST 94[35] estimate to which Dorofeeva's increments for 1,3-Cl interaction[39] were added (see Tables 51 and 52).

7.26. $C_{12}H_5Cl_4O_3\cdot$ (1,3-dichloro-1-ol-2-yl-3,5,-cyclohexadiene-*p*-dioxin-6,8-dichlorobenzen radical)

It is not clear whether this radical really exists or it is only a transition state. Nevertheless the PM3, PM3 UHF, AM1, and AM1 UHF were successful calculations. A very rough estimate of its enthalpy of formation was made according to Dorofeeva[39] and Bozzelli's[46] increments (see Tables 53 and 54).

7.27. $\cdot C_{12}H_5Cl_4O_3$ (1,3,-dichloro-2-ol-3-yl-1,4-cyclohexadiene-*p*-dioxin-6,8-dichlorobenzene radical)

This is a second configuration of the former (7.26) radical. The PM3, PM3, UHF, and AM1 UHF were successful. The AM1 failed. A very rough estimate of its enthalpy of formation was made using Dorofeeva's[39] and Bozzelli's[46] increments (see Tables 55 and 56).

7.28. $C_{12}H_5Cl_5O_2$ (2,4-dichlorophenol-1′,3′,5′-trichlorophenyl-6-6′-ether-$Cl_2C_6H_2(OH)-O-C_6H_2Cl_3$) (PD)

This chloro phenyl-phenol ether that belongs to the group of compounds known in the literature under the abbreviation PD, was calculated using the MOPAC PM3 method. Its enthalpy of formation was estimated using the NIST 94[35] estimate + the Dorofeeva[39] 1,3-Cl corrections + the Bozzelli ortho Cl–OH corrections (Wu *et al.*[46]) (see Tables 57 and 58).

TABLE 22. Thermodynamic properties of $C_6H_4ClO\cdot$ (o-chlorophenoxy radical) (M_r=127.550)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	C_p° ($J\cdot K^{-1}\cdot mol^{-1}$)	$H°-H°(T_r)$ ($J\cdot mol^{-1}$)	$S°$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$-[G°-H°(T_r)]/T$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$H(T)$ ($kJ\cdot mol^{-1}$)	$\Delta_f H°$ ($kJ\cdot mol^{-1}$)	log K_f
0	—	−19.751	—	—	−1.760	30.428	—
100	50.545	−15.788	267.573	425.453	2.203	25.118	−19.4234
200	79.670	−9.311	311.314	357.867	8.681	21.271	−13.2694
298.15	109.954	0.000	348.788	348.788	17.991	17.991	−11.5664
300	110.511	0.204	349.470	348.790	18.195	17.935	−11.5469
400	138.559	12.695	385.210	353.473	30.686	15.255	−10.8214
500	161.671	27.748	418.705	363.208	45.740	13.188	−10.4493
600	180.123	44.873	449.876	375.088	62.864	11.594	−10.2331
700	194.896	63.650	478.792	387.863	81.642	10.397	−10.0963
800	206.885	83.760	505.626	400.927	101.751	9.554	−10.0035
900	216.751	104.957	530.582	413.963	122.948	9.032	−9.9362
1000	224.962	127.055	553.857	426.802	145.046	8.778	−9.8846
1100	231.854	149.905	575.630	439.353	167.897	8.756	−9.8430
1200	237.682	173.390	596.061	451.569	191.381	8.922	−9.8081
1300	242.640	197.413	615.287	463.431	215.404	9.236	−9.7780
1400	246.880	221.894	633.428	474.932	239.886	9.650	−9.7506
1500	250.526	246.769	650.588	486.075	264.760	10.154	−9.7264
1600	253.677	271.983	666.860	496.870	289.974	10.706	−9.7038
1700	256.413	297.491	682.323	507.328	315.482	11.284	−9.6827
1800	258.799	323.254	697.048	517.463	341.245	11.873	−9.6629
1900	260.890	349.241	711.098	527.287	367.232	12.456	−9.6443
2000	262.731	375.424	724.528	536.816	393.415	13.021	−9.6266
2100	264.357	401.780	737.386	546.063	419.771	13.558	−9.6102
2200	265.800	428.289	749.718	555.041	446.280	14.046	−9.5945
2300	267.084	454.934	761.562	563.765	472.926	14.493	−9.5798
2400	268.233	481.701	772.954	572.245	499.693	14.883	−9.5662
2500	269.263	508.577	783.925	580.494	526.568	15.199	−9.5528
2600	270.189	535.550	794.504	588.523	553.542	15.457	−9.5404
2700	271.026	562.612	804.717	596.342	580.603	15.634	−9.5290
2800	271.783	589.753	814.588	603.962	607.744	15.734	−9.5183
2900	272.471	616.966	824.137	611.390	634.958	15.751	−9.5080
3000	273.097	644.245	833.385	618.637	662.236	15.669	−9.4983
3100	273.668	671.584	842.349	625.709	689.575	15.516	−9.4899
3200	274.191	698.977	851.046	632.616	716.968	15.260	−9.4817
3300	274.671	726.421	859.491	639.364	744.412	14.912	−9.4742
3400	275.111	753.910	867.697	645.959	771.901	14.471	−9.4673
3500	275.517	781.442	875.678	652.409	799.433	13.927	−9.4612
3600	275.892	809.013	883.445	658.719	827.004	13.295	−9.4554
3700	276.239	836.619	891.009	664.896	854.611	12.559	−9.4505
3800	276.560	864.259	898.380	670.943	882.251	11.728	−9.4458
3900	276.858	891.931	905.568	676.868	909.922	10.805	−9.4420
4000	277.135	919.630	912.581	682.673	937.622	9.774	−9.4383
4100	277.393	947.357	919.427	688.365	965.348	8.664	−9.4356
4200	277.634	975.108	926.115	693.946	993.100	7.455	−9.4332
4300	277.858	1002.883	932.650	699.421	1020.874	6.147	−9.4310
4400	278.069	1030.680	939.040	704.795	1048.671	4.732	−9.4292
4500	278.266	1058.496	945.292	710.070	1076.487	3.246	−9.4282
4600	278.451	1086.332	951.410	715.250	1104.323	1.677	−9.4276
4700	278.624	1114.186	957.400	720.339	1132.177	0.030	−9.4274
4800	278.787	1142.057	963.268	725.339	1160.048	−1.696	−9.4278
4900	278.941	1169.943	969.018	730.254	1187.934	−3.498	−9.4285
5000	279.086	1197.845	974.654	735.086	1215.836	−5.434	−9.4291
5100	279.223	1225.760	980.182	739.837	1243.751	−7.375	−9.4309
5200	279.352	1253.689	985.606	744.512	1271.680	−9.427	−9.4325
5300	279.474	1281.630	990.928	749.111	1299.621	−11.552	−9.4345
5400	279.590	1309.584	996.153	753.638	1327.575	−13.748	−9.4368
5500	279.699	1337.548	1001.284	758.094	1355.539	−16.012	−9.4395
5600	279.803	1365.523	1006.325	762.482	1383.514	−18.346	−9.4423
5700	279.902	1393.508	1011.278	766.803	1411.500	−20.744	−9.4456
5800	279.995	1421.503	1016.147	771.060	1439.494	−23.207	−9.4491
5900	280.084	1449.507	1020.934	775.255	1467.499	−25.731	−9.4527
6000	280.169	1477.520	1025.642	779.389	1495.511	−28.314	−9.4567

TABLE 23. Molecular properties of $\cdot C_6H_4ClO$ (2,5-cyclohexadiene-2-chloro-1-one-4-yl). Values listed with bold characters were chosen for thermodynamic calculations—$\sigma = \mathbf{1}$ and statistical weight $= \mathbf{2}$

	Enthalpy of formation $\Delta_f H°(298.15\ \text{K})$ / kcal mol^{-1}			Zero point energy ZPE / kcal mol^{-1}	
Therm[14]	**16.19±15**				
PM3	6.56			51.203	
PM3 UHF	−3.621			50.552	
AM1	9.48			53.328	
	Moments of inertia of the molecule / g cm^2×10^{-39}				
MOPAC method	I_a		I_b		I_c
PM3	**27.258 929**		**53.038 78**		**80.277 364**
PM3 UHF	27.322 419		53.516 78		80.838 894
AM1	27.666 032		53.501 41		81.164 006
	Molecular vibrations / cm^{-1}				
PM3	**88.5**	**218**	**247**	**370**	**412**	**432**
	522	**554**	**689**	**698**	**778**	**869**
	870	**959**	**1001**	**1025**	**1089**	**1132**
	1151	**1178**	**1269**	**1392**	**1419**	**1602**
	1746	**1869**	**3048**	**3050**	**3065**	**3075**
PM3 UHF	85.6	207	243	374	389	410
	519	546	667	679	747	837
	860	905	947	1026	1092	1123
	1147	1187	1379	1391	1412	1567
	1610	1777	3049	3052	3064	3073
AM1	90.2	220	269	411	421	435
	550	588	710	765	801	898
	923	960	990	1126	1152	1193
	1228	1265	1323	1430	1468	1617
	1740	1932	3191	3194	3203	3211

7.29. $C_{12}H_6Cl_4O_2$ (2,4-dichlorophenol-1′,3′-dichlorophenyl-6-2′-ether)

It is not clear that this species exists. Only PM3 calculations were successful, AM1 calculation resulted in a transition state and the PM3 UHF and AM1 UHF calculations, both failed. Like the PD species we roughly estimated the enthalpy of formation by calculating the NIST 94[35] estimate and correcting it for the 1,3 Cl interaction according to Dorofeeva *et al.*[39] and the Cl–OH interaction according to Bozzelli[46] (see Tables 59 and 60).

7.30. $C_{12}H_8O$ (dibenzofuran) (DF)

Dibenzofuran was calculated by Dorofeeva *et al.*,[39] using group additivity methods. In our case the species was calculated from experimental vibrations supplied by Dorofeeva[48] and the enthalpy of formation supplied by Chirico.[52] $\Delta_f H°(298.15\ \text{K}) = 55.2\ \text{kJ mol}^{-1}$.[39] The IR spectrum[26] was published after the revisions to this paper were finished (see Tables 61 and 62).

7.31. $C_{12}H_8O_2$ (dibenzo-*p*-dioxin) (DD)

This compound was published by Dorofeeva *et al.*[39] based on group additivity methods. The species here is calculated using experimental vibrations supplied by Dorofeeva,[48] and her calculated moments of inertia. The PM3 calculations are brought for comparison purposes.

The enthalpy of formation is estimated by Dorofeeva *et al.*[39] and recommended by NIST 2000[26,62] $\Delta_f H°(298.15\ \text{K})/\text{kJ mol}^{-1} = -59.2 \pm 3.8$ (see Tables 63 and 64).

TABLE 24. Thermodynamic properties of ·C_6H_4ClO (2,5-cyclohexadiene-2-chloro-1-one-4-yl) (M_r=127.550)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	C_p° (J·K^{-1}·mol^{-1})	$H°-H°(T_r)$ (J·mol^{-1})	$S°$ (J·K^{-1}·mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}·mol^{-1})	$H(T)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	log K_f
0	—	−19.797	—	—	47.942	80.130	—
100	50.744	−15.802	262.514	420.530	51.937	74.852	−45.6655
200	79.726	−9.313	306.336	352.903	58.426	71.016	−26.5212
298.15	109.949	0.000	343.821	343.821	67.739	67.739	−20.5412
300	110.505	0.204	344.503	343.824	67.943	67.683	−20.4680
400	138.454	12.689	380.229	348.505	80.428	64.997	−17.5771
500	161.461	27.727	413.689	358.235	95.466	62.914	−15.9061
600	179.840	44.827	444.815	370.103	112.566	61.295	−14.8243
700	194.577	63.574	473.684	382.864	131.313	60.068	−14.0696
800	206.559	83.651	500.475	395.912	151.390	59.193	−13.5136
900	216.434	104.816	525.393	408.931	172.555	58.639	−13.0863
1000	224.662	126.883	548.635	421.752	194.622	58.354	−12.7468
1100	231.576	149.704	570.381	434.286	217.443	58.302	−12.4700
1200	237.427	173.162	590.788	446.486	240.901	58.442	−12.2390
1300	242.406	197.161	609.995	458.333	264.900	58.731	−12.0431
1400	246.667	221.620	628.119	469.819	289.359	59.123	−11.8737
1500	250.332	246.474	645.265	480.949	314.213	59.607	−11.7265
1600	253.500	271.670	661.525	491.731	339.409	60.141	−11.5963
1700	256.251	297.160	676.978	502.177	364.899	60.702	−11.4802
1800	258.651	322.908	691.694	512.301	390.647	61.275	−11.3761
1900	260.754	348.881	705.736	522.115	416.620	61.844	−11.2821
2000	262.605	375.050	719.159	531.634	442.789	62.396	−11.1965
2100	264.241	401.394	732.012	540.872	469.133	62.920	−11.1187
2200	265.692	427.893	744.339	549.842	495.631	63.398	−11.0472
2300	266.985	454.528	756.178	558.557	522.267	63.834	−10.9816
2400	268.141	481.285	767.566	567.030	549.024	64.214	−10.9212
2500	269.177	508.152	778.533	575.273	575.891	64.521	−10.8650
2600	270.109	535.117	789.109	583.295	602.856	64.771	−10.8130
2700	270.951	562.171	799.319	591.108	629.910	64.941	−10.7649
2800	271.713	589.305	809.187	598.721	657.043	65.033	−10.7201
2900	272.405	616.511	818.734	606.144	684.250	65.043	−10.6780
3000	273.035	643.784	827.980	613.385	711.522	64.955	−10.6387
3100	273.610	671.116	836.942	620.453	738.855	64.796	−10.6026
3200	274.136	698.504	845.637	627.355	766.243	64.534	−10.5686
3300	274.619	725.942	854.080	634.098	793.681	64.181	−10.5366
3400	275.063	753.426	862.285	640.689	821.165	63.736	−10.5068
3500	275.471	780.953	870.265	647.135	848.692	63.186	−10.4791
3600	275.848	808.520	878.030	653.441	876.259	62.549	−10.4529
3700	276.197	836.122	885.593	659.614	903.861	61.810	−10.4286
3800	276.520	863.758	892.963	665.655	931.497	60.975	−10.4056
3900	276.820	891.425	900.150	671.579	959.164	60.048	−10.3845
4000	277.099	919.121	907.162	677.381	986.860	59.013	−10.3643
4100	277.359	946.845	914.007	683.070	1014.583	57.900	−10.3460
4200	277.601	974.593	920.694	688.648	1042.332	56.687	−10.3286
4300	277.827	1002.364	927.229	694.121	1070.103	55.376	−10.3122
4400	278.039	1030.158	933.618	699.492	1097.897	53.958	−10.2968
4500	278.237	1057.971	939.869	704.764	1125.710	52.469	−10.2828
4600	278.423	1085.805	945.986	709.942	1153.544	50.897	−10.2697
4700	278.598	1113.656	951.976	715.028	1181.395	49.247	−10.2576
4800	278.762	1141.524	957.843	720.026	1209.263	47.519	−10.2467
4900	278.917	1169.408	963.593	724.938	1237.147	45.715	−10.2365
5000	279.063	1197.307	969.229	729.768	1265.046	43.775	−10.2266
5100	279.200	1225.220	974.756	734.517	1292.959	41.833	−10.2183
5200	279.330	1253.147	980.179	739.190	1320.886	39.778	−10.2102
5300	279.453	1281.086	985.501	743.787	1348.825	37.652	−10.2029
5400	279.569	1309.037	990.726	748.312	1376.776	35.454	−10.1962
5500	279.680	1337.000	995.857	752.766	1404.738	33.187	−10.1902
5600	279.784	1364.973	1000.897	757.152	1432.712	30.852	−10.1847
5700	279.883	1392.956	1005.850	761.472	1460.695	28.451	−10.1799
5800	279.978	1420.949	1010.719	765.727	1488.688	25.987	−10.1756
5900	280.067	1448.952	1015.505	769.920	1516.691	23.461	−10.1718
6000	280.153	1476.963	1020.213	774.053	1544.702	20.876	−10.1685

TABLE 25. Molecular properties of $\cdot C_6H_4ClO$ (2,4-cyclohexadiene-6-chloro-1-one-2-yl). Values listed with bold characters were chosen for thermodynamic calculations—$\sigma = \mathbf{1}$ and statistical weight $= \mathbf{2}$

MOPAC method	Enthalpy of formation $\Delta_f H°(298.15\ K)$ / kcal mol^{-1}	Zero point energy ZPE / kcal mol^{-1}
Our estimate	**55.0±30**	
PM3	44.97	51.520
PM3 UHF	36.68	50.390
AM1	49.90	53.664

Moments of inertia of the molecule / g cm^2×10^{-39}

MOPAC method	I_a	I_b	I_c
PM3	**31.083 57**	**49.937 92**	**74.566 00**
PM3 UHF	31.066 28	49.999 49	74.633 86
AM1	31.332 85	49.856 11	74.861 38

Molecular vibrations / cm^{-1}

PM3	**54.3**	**199.4**	**214**	**339**	**429**	**462**
	503	**577**	**632**	**752**	**829**	**840**
	908	**940**	**994**	**1022**	**1073**	**1122**
	1131	**1147**	**1297**	**1315**	**1416**	**1824**
	1914	**1986**	**2906**	**3048**	**3073**	**3094**
PM3 UHF	47.7	164	207	316	403	454
	494	562	619	730	797	830
	856	922	955	1010	1066	1111
	1124	1141	1280	1299	1368	1605
	1823	1964	2904	3045	3068	3085
AM1	36	220	240	360	431	490
	527	605	706	783	870	896
	937	987	1012	1090	1138	1155
	1192	1213	1359	1360	1441	1883
	1919	2017	3046	3191	3211	3226

TABLE 26. Thermodynamic properties of $\cdot C_6H_4ClO$ (2,4-cyclohexadiene-6-chloro-1-one-2-yl) (M_r=127.550)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	C_p° ($J\cdot K^{-1}\cdot mol^{-1}$)	$H°-H°(T_r)$ ($J\cdot mol^{-1}$)	$S°$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$-[G°-H°(T_r)]/T$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$H(T)$ ($kJ\cdot mol^{-1}$)	$\Delta_f H°$ ($kJ\cdot mol^{-1}$)	log K_f
0	—	−20.158	—	—	209.962	242.149	—
100	52.759	−15.961	267.165	426.773	214.159	237.074	−130.1564
200	80.356	−9.349	311.903	358.646	220.771	233.362	−68.6297
298.15	110.114	0.000	349.538	349.538	230.120	230.120	−48.6903
300	110.664	0.204	350.221	349.540	230.324	230.064	−48.4417
400	138.280	12.689	385.948	354.224	242.809	227.378	−38.4827
500	160.972	27.693	419.334	363.947	257.813	225.261	−32.5711
600	179.153	44.733	450.350	375.795	274.853	223.582	−28.6631
700	193.816	63.407	479.107	388.526	293.527	222.282	−25.8906
800	205.806	83.407	505.796	401.537	313.527	221.330	−23.8219
900	215.733	104.499	530.628	414.517	334.619	220.704	−22.2186
1000	224.030	126.500	553.800	427.300	356.620	220.352	−20.9387
1100	231.016	149.262	575.489	439.796	379.382	220.241	−19.8928
1200	236.933	172.667	595.851	451.961	402.787	220.328	−19.0211
1300	241.972	196.619	615.020	463.774	426.739	220.571	−18.2833
1400	246.286	221.038	633.114	475.230	451.158	220.922	−17.6494
1500	249.996	245.856	650.235	486.331	475.976	221.370	−17.0998
1600	253.202	271.020	666.475	497.087	501.140	221.872	−16.6176
1700	255.986	296.483	681.910	507.509	526.603	222.405	−16.1910
1800	258.415	322.205	696.612	517.609	552.325	222.954	−15.8109
1900	260.542	348.155	710.642	527.403	578.275	223.500	−15.4700
2000	262.414	374.305	724.055	536.902	604.425	224.032	−15.1621
2100	264.069	400.631	736.899	546.122	630.751	224.538	−14.8834
2200	265.536	427.113	749.218	555.076	657.233	224.999	−14.6292
2300	266.842	453.733	761.051	563.776	683.853	225.420	−14.3967
2400	268.010	480.477	772.433	572.234	710.597	225.787	−14.1835
2500	269.057	507.331	783.395	580.463	737.451	226.081	−13.9865
2600	269.999	534.284	793.967	588.473	764.404	226.320	−13.8047
2700	270.849	561.328	804.173	596.273	791.448	226.479	−13.6364
2800	271.619	588.452	814.037	603.876	818.572	226.561	−13.4800
2900	272.317	615.649	823.581	611.288	845.769	226.562	−13.3341
3000	272.953	642.913	832.824	618.519	873.033	226.465	−13.1978
3100	273.534	670.238	841.783	625.578	900.358	226.298	−13.0710
3200	274.065	697.618	850.476	632.470	927.738	226.029	−12.9519
3300	274.552	725.049	858.917	639.205	955.169	225.670	−12.8401
3400	274.999	752.527	867.120	645.789	982.647	225.217	−12.7350
3500	275.412	780.048	875.098	652.227	1010.168	224.661	−12.6365
3600	275.792	807.608	882.862	658.526	1037.728	224.019	−12.5433
3700	276.144	835.205	890.423	664.692	1065.325	223.274	−12.4558
3800	276.470	862.836	897.792	670.729	1092.956	222.434	−12.3728
3900	276.772	890.499	904.977	676.644	1120.619	221.502	−12.2947
4000	277.054	918.190	911.988	682.440	1148.310	220.462	−12.2205
4100	277.316	945.909	918.832	688.123	1176.029	219.345	−12.1507
4200	277.560	973.653	925.518	693.696	1203.773	218.128	−12.0844
4300	277.788	1001.420	932.052	699.163	1231.540	216.813	−12.0213
4400	278.002	1029.210	938.440	704.529	1259.330	215.391	−11.9613
4500	278.202	1057.020	944.690	709.797	1287.140	213.899	−11.9048
4600	278.389	1084.850	950.807	714.970	1314.970	212.323	−11.8510
4700	278.565	1112.698	956.796	720.052	1342.818	210.670	−11.7999
4800	278.731	1140.562	962.662	725.045	1370.682	208.939	−11.7515
4900	278.887	1168.443	968.411	729.953	1398.563	207.131	−11.7054
5000	279.034	1196.340	974.047	734.779	1426.460	205.189	−11.6611
5100	279.173	1224.250	979.574	739.525	1454.370	203.244	−11.6198
5200	279.304	1252.174	984.996	744.194	1482.294	201.187	−11.5799
5300	279.428	1280.111	990.318	748.787	1510.231	199.058	−11.5420
5400	279.545	1308.059	995.542	753.309	1538.179	196.857	−11.5059
5500	279.656	1336.019	1000.672	757.760	1566.139	194.588	−11.4715
5600	279.762	1363.990	1005.712	762.142	1594.110	192.250	−11.4386
5700	279.862	1391.972	1010.665	766.459	1622.092	189.848	−11.4074
5800	279.957	1419.962	1015.533	770.712	1650.082	187.381	−11.3776
5900	280.047	1447.963	1020.319	774.902	1678.083	184.853	−11.3492
6000	280.133	1475.972	1025.027	779.032	1706.092	182.267	−11.3221

TABLE 27. Molecular properties of $C_6H_4Cl_2O$ (2,4-dichlorophenol). Values listed with bold characters were chosen for thermodynamic calculations—$\sigma = \mathbf{1}$ and statistical weight = **1**

	Enthalpy of formation $\Delta_f H°(298.15\ \text{K})$ / kcal mol^{-1}	Zero point energy ZPE / kcal mol^{-1}
DaSilva[43]	**−37.356±0.45**	
Thergas[37]	−35.28[a]; −33.61[b]	
PM3	−33.22	54.165
PM3 UHF	−33.32	53.801
AM1	−32.37	55.561
AM1 UHF	−32.74	55.081

[a]Benson's method.
[b]Yoneda's method.

Moments of inertia of the molecule / g cm$^2 \times 10^{-39}$

MOPAC method	I_a	I_b	I_c
PM3	**39.337 99**	**97.932 12**	**137.269 994**
PM3 UHF	39.362 810	98.027 240	137.390 046
AM1	39.520 133	99.691 264	139.211 394
AM1 UHF	39.553 990	99.881 983	139.435 969

Reduced moment of inertia[34] $I_r = \mathbf{0.1364}$ g cm$^2 \times 10^{-39}$; $\sigma = \mathbf{2}$; $V(2) = \mathbf{1116.8}$ cm^{-1}.

Molecular vibrations / cm^{-1}

Ir[26]				**509**	**551**	**656**
	726	**772**	**813**	**866**	**939**	**1058**
	1079	**1097**	**1191**	**1282**	**1331**	**1408**
	1481	**1582**	**1628**	**1736**	**1876**	**3078**
	3302	**3582**	**3651**			
PM3	95.0	**184**	**203**	**277**	**285**	**306**
	366	**403**	**482**	514	533	616
	741	771	814	874	931	999
	1089	1141	1159	1195	1301	1393
	1426	1557	1611	1775	1782	3054
	3058	3076	3858			
PM3 UHF	92	183	202	268	285	288
	366	402	474	508	532	613
	728	770	803	869	919	985
	1084	1140	1157	1170	1301	1376
	1419	1546	1595	1744	1748	3056
	3061	3076	3858			
AM1	89.8	188	219	273	298	301
	413	443	393	545	566	681
	731	840	884	933	953	995
	1180	1205	1253	1293	1361	1464
	1475	1598	1666	1760	1764	3178
	3179	3197	3408			
AM1 UHF	87	180	218	264	291	300
	411	441	476	530	563	677
	705	823	882	924	932	975
	1175	1206	1251	1268	1379	1446
	1474	1584	1647	1714	1731	3180
	3181	3196	3410			

TABLE 28. Thermodynamic properties of $C_6H_4Cl_2O$ (2-4-dichlorophenol) (M_r=163.003)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	C_p° ($J\cdot K^{-1}\cdot mol^{-1}$)	$H°-H°(T_r)$ ($J\cdot mol^{-1}$)	$S°$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$-[G°-H°(T_r)]/T$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$H(T)$ ($kJ\cdot mol^{-1}$)	$\Delta_f H°$ ($kJ\cdot mol^{-1}$)	log K_f
0	—	−22.740	—	—	−179.040	−142.262	—
100	54.866	−18.831	269.293	457.601	−175.131	−149.081	66.7203
200	96.598	−11.190	320.589	376.537	−167.490	−153.284	27.3193
298.15	130.408	0.000	365.660	365.660	−156.300	−156.300	14.0231
300	130.988	0.242	366.469	365.663	−156.058	−156.350	13.8543
400	159.360	14.808	408.178	371.158	−141.492	−158.690	7.0004
500	182.088	31.925	446.278	382.429	−124.375	−160.479	2.8331
600	200.043	51.066	481.128	396.017	−105.234	−161.872	0.0274
700	214.324	71.811	513.078	410.491	−84.489	−162.938	−1.9923
800	225.875	93.841	542.477	425.176	−62.459	−163.711	−3.5159
900	235.389	116.918	569.648	439.738	−39.382	−164.211	−4.7055
1000	243.344	140.866	594.872	454.006	−15.434	−164.484	−5.6593
1100	250.075	165.547	618.390	467.893	9.247	−164.553	−6.4406
1200	255.820	190.849	640.402	481.361	34.549	−164.450	−7.0916
1300	260.758	216.684	661.078	494.398	60.384	−164.210	−7.6421
1400	265.027	242.978	680.562	507.007	86.678	−163.875	−8.1126
1500	268.734	269.670	698.977	519.197	113.370	−163.449	−8.5201
1600	271.969	296.709	716.426	530.983	140.409	−162.972	−8.8754
1700	274.802	324.051	733.001	542.383	167.751	−162.465	−9.1879
1800	277.294	351.658	748.780	553.415	195.358	−161.942	−9.4648
1900	279.493	379.500	763.833	564.096	223.200	−161.419	−9.7117
2000	281.442	407.548	778.220	574.445	251.248	−160.908	−9.9330
2100	283.175	435.781	791.994	584.479	279.481	−160.422	−10.1330
2200	284.720	464.177	805.204	594.214	307.877	−159.981	−10.3140
2300	286.104	492.720	817.891	603.665	336.420	−159.579	−10.4789
2400	287.346	521.393	830.094	612.847	365.093	−159.235	−10.6300
2500	288.464	550.185	841.847	621.773	393.885	−158.966	−10.7683
2600	289.475	579.082	853.181	630.457	422.782	−158.759	−10.8959
2700	290.390	608.076	864.123	638.910	451.776	−158.639	−11.0141
2800	291.221	637.158	874.699	647.143	480.858	−158.603	−11.1239
2900	291.978	666.318	884.932	655.167	510.018	−158.659	−11.2257
3000	292.668	695.551	894.842	662.992	539.251	−158.824	−11.3207
3100	293.300	724.850	904.449	670.627	568.550	−159.072	−11.4103
3200	293.880	754.209	913.771	678.080	597.909	−159.435	−11.4941
3300	294.412	783.624	922.822	685.360	627.324	−159.903	−11.5730
3400	294.902	813.090	931.618	692.474	656.790	−160.476	−11.6475
3500	295.355	842.603	940.174	699.430	686.303	−161.167	−11.7183
3600	295.773	872.160	948.500	706.233	715.860	−161.958	−11.7851
3700	296.161	901.757	956.609	712.891	745.457	−162.863	−11.8489
3800	296.520	931.391	964.512	719.409	775.091	−163.875	−11.9094
3900	296.854	961.060	972.219	725.793	804.760	−164.988	−11.9675
4000	297.165	990.761	979.738	732.048	834.461	−166.218	−12.0228
4100	297.455	1020.493	987.080	738.179	864.193	−167.532	−12.0762
4200	297.726	1050.252	994.251	744.191	893.952	−168.951	−12.1273
4300	297.979	1080.037	1001.260	750.088	923.737	−170.471	−12.1761
4400	298.216	1109.847	1008.113	755.875	953.547	−172.098	−12.2231
4500	298.438	1139.680	1014.817	761.555	983.380	−173.796	−12.2688
4600	298.647	1169.534	1021.379	767.132	1013.234	−175.575	−12.3128
4700	298.843	1199.409	1027.803	772.610	1043.109	−177.427	−12.3555
4800	299.027	1229.302	1034.097	777.992	1073.002	−179.350	−12.3970
4900	299.201	1259.214	1040.265	783.282	1102.914	−181.343	−12.4372
5000	299.365	1289.142	1046.311	788.483	1132.842	−183.460	−12.4757
5100	299.520	1319.086	1052.241	793.596	1162.786	−185.570	−12.5140
5200	299.666	1349.046	1058.058	798.626	1192.746	−187.779	−12.5507
5300	299.804	1379.019	1063.768	803.575	1222.719	−190.046	−12.5865
5400	299.936	1409.006	1069.373	808.446	1252.706	−192.370	−12.6215
5500	300.060	1439.006	1074.878	813.240	1282.706	−194.747	−12.6555
5600	300.178	1469.018	1080.285	817.961	1312.718	−197.175	−12.6887
5700	300.290	1499.042	1085.599	822.610	1342.742	−199.651	−12.7212
5800	300.396	1529.076	1090.823	827.189	1372.776	−202.173	−12.7530
5900	300.497	1559.121	1095.959	831.701	1402.821	−204.738	−12.7840
6000	300.594	1589.175	1101.010	836.148	1432.875	−207.341	−12.8144

TABLE 29. Molecular properties of C_6H_5ClO (o-chlorophenol). Values listed with bold characters were chosen for thermodynamic calculations—$\sigma = \mathbf{1}$ and statistical weight = **1**

	Enthalpy of formation $\Delta_f H°(298.15\ \text{K})$ / kcal mol^{-1}	Zero point energy ZPE / kcal mol^{-1}
NIST 94[35]	**−29.4±1.0**	
Shaub[36]	−31.11	
Thergas[37]	−27.91[a]; −27.97[b]	
PM3	−28.15	59.905
AM1	−28.666	61.390
AM1 UHF	−28.84	61.050

[a]Benson's method.
[b]Yoneda's method.

Moments of inertia of the molecule / g cm$^2 \times 10^{-39}$

MOPAC method	I_a	I_b	I_c
PM3	**28.5786**	**53.444 47**	**82.023 07**
AM1	28.89843	54.041 4	82.939 83
AM1 UHF	28.96205	54.087 3	83.049 36

Reduced moment of inertia[34] $I_r = \mathbf{0.1364}$ g cm$^2 \times 10^{-39}$; $\sigma = \mathbf{2}$; $V(2) = \mathbf{1116.8}$ cm^{-1}.

Molecular vibrations / cm^{-1}

Ir[26]		**494**	**553**	**680**		**746**
	842		**924**	**1027**	**1054**	**1125**
	1196	**1245**	**1288**	**1326**	**1381**	**1479**
		1588	**1669**	**1767**	**3052**	**3084**
	3326	**3569**	**3650**			
PM3	137	**247.5**	**263**	**299**	**378**	**421**
	487	496	564	697	**703**	782
	875	**890**	961	1007	1073	1114
	1151	1168	1195	1294	1395	1423
	1565	1609	1779	1789	3055	3060
	3069	3079	3859			
AM1	138.6	256	262	305	412	445
	497	523	601	700	770	818
	913	934	972	1000	1155	1175
	1201	1252	1282	1362	1472	1475
	1603	1667	1770	1775	3183	3186
	3195	3202	3421			
AM1 UHF	135.6	250	261.5	299	410	436
	485	521	598	684	766	807
	899	928	958	986	1151	1168
	1199	1234	1279	1370	1458	1471
	1591	1653	1734	1742	3185	3186
	3195	3202	3422			

TABLE 30. Thermodynamic properties of C_6H_5ClO (o-chlorophenol) (M_r=128.557)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	C_p° ($J\cdot K^{-1}\cdot mol^{-1}$)	$H°-H°(T_r)$ ($J\cdot mol^{-1}$)	$S°$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$-[G°-H°(T_r)]/T$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$H(T)$ ($kJ\cdot mol^{-1}$)	$\Delta_f H°$ ($kJ\cdot mol^{-1}$)	log K_f
0	—	−20.507	—	—	−143.517	−107.095	—
100	47.903	−16.844	256.988	425.428	−139.854	−114.204	50.1657
200	86.240	−10.104	302.172	352.690	−133.113	−119.135	19.8038
298.15	118.897	0.000	342.841	342.841	−123.010	−123.010	9.4122
300	119.471	0.220	343.578	342.843	−122.789	−123.075	9.2793
400	148.002	13.636	381.974	347.885	−109.374	−126.284	3.8564
500	171.422	29.649	417.610	358.312	−93.361	−128.853	0.5258
600	190.178	47.764	450.586	370.979	−75.246	−130.921	−1.7350
700	205.252	67.562	481.075	384.557	−55.448	−132.566	−3.3732
800	217.567	88.723	509.313	398.409	−34.287	−133.834	−4.6158
900	227.805	111.006	535.547	412.207	−12.003	−134.756	−5.5901
1000	236.440	134.231	560.008	425.778	11.221	−135.387	−6.3740
1100	243.798	158.252	582.897	439.032	35.242	−135.758	−7.0179
1200	250.117	182.956	604.388	451.925	59.946	−135.911	−7.5554
1300	255.574	208.247	624.629	464.439	85.237	−135.890	−8.0108
1400	260.309	234.046	643.747	476.571	111.037	−135.739	−8.4002
1500	264.434	260.288	661.850	488.325	137.279	−135.473	−8.7379
1600	268.041	286.916	679.034	499.711	163.906	−135.132	−9.0326
1700	271.207	313.882	695.381	510.745	190.872	−134.742	−9.2916
1800	273.996	341.145	710.963	521.438	218.135	−134.321	−9.5213
1900	276.461	368.670	725.845	531.808	245.660	−133.885	−9.7261
2000	278.647	396.428	740.082	541.868	273.418	−133.450	−9.9096
2100	280.592	424.391	753.725	551.634	301.382	−133.029	−10.0755
2200	282.329	452.539	766.819	561.120	329.529	−132.641	−10.2256
2300	283.884	480.851	779.404	570.338	357.842	−132.283	−10.3623
2400	285.282	509.311	791.516	579.303	386.301	−131.971	−10.4876
2500	286.541	537.903	803.188	588.027	414.893	−131.724	−10.6021
2600	287.678	566.615	814.449	596.520	443.605	−131.526	−10.7078
2700	288.709	595.435	825.326	604.794	472.425	−131.402	−10.8058
2800	289.645	624.353	835.842	612.859	501.344	−131.349	−10.8967
2900	290.498	653.361	846.021	620.725	530.352	−131.374	−10.9810
3000	291.276	682.450	855.883	628.400	559.441	−131.494	−11.0596
3100	291.989	711.614	865.446	635.893	588.605	−131.681	−11.1339
3200	292.642	740.846	874.727	643.212	617.837	−131.969	−11.2032
3300	293.242	770.141	883.741	650.365	647.131	−132.346	−11.2685
3400	293.795	799.493	892.503	657.358	676.483	−132.815	−11.3302
3500	294.306	828.898	901.027	664.199	705.889	−133.388	−11.3888
3600	294.778	858.353	909.325	670.893	735.343	−134.048	−11.4440
3700	295.215	887.853	917.407	677.447	764.843	−134.811	−11.4969
3800	295.620	917.395	925.286	683.866	794.385	−135.671	−11.5470
3900	295.997	946.976	932.970	690.155	823.966	−136.624	−11.5951
4000	296.348	976.593	940.468	696.320	853.584	−137.688	−11.6408
4100	296.675	1006.245	947.790	702.364	883.235	−138.831	−11.6851
4200	296.981	1035.928	954.943	708.293	912.918	−140.077	−11.7275
4300	297.267	1065.640	961.934	714.111	942.631	−141.424	−11.7679
4400	297.534	1095.381	968.771	719.821	972.371	−142.881	−11.8069
4500	297.785	1125.147	975.461	725.428	1002.137	−144.412	−11.8448
4600	298.021	1154.937	982.008	730.935	1031.927	−146.031	−11.8814
4700	298.242	1184.750	988.420	736.345	1061.741	−147.730	−11.9169
4800	298.450	1214.585	994.701	741.662	1091.575	−149.511	−11.9515
4900	298.646	1244.440	1000.857	746.890	1121.430	−151.373	−11.9851
5000	298.832	1274.314	1006.892	752.029	1151.304	−153.373	−12.0172
5100	299.006	1304.206	1012.812	757.085	1181.196	−155.381	−12.0494
5200	299.172	1334.115	1018.619	762.059	1211.105	−157.503	−12.0801
5300	299.328	1364.040	1024.320	766.954	1241.030	−159.702	−12.1102
5400	299.476	1393.980	1029.916	771.772	1270.971	−161.976	−12.1396
5500	299.616	1423.935	1035.412	776.515	1300.925	−164.322	−12.1683
5600	299.750	1453.903	1040.812	781.187	1330.894	−166.739	−12.1963
5700	299.876	1483.885	1046.119	785.788	1360.875	−169.223	−12.2238
5800	299.996	1513.878	1051.335	790.322	1390.869	−171.775	−12.2508
5900	300.110	1543.884	1056.465	794.789	1420.874	−174.390	−12.2771
6000	300.219	1573.900	1061.509	799.193	1450.891	−177.066	−12.3031

TABLE 31. Molecular properties of $\cdot C_6H_5O$ (2,4-cyclohexadiene-1-one-2-yl radical). Values listed with bold characters were chosen for thermodynamic calculations—$\sigma = \mathbf{1}$ and statistical weight $= \mathbf{2}$

	Enthalpy of formation $\Delta_f H°(298.15\ \mathrm{K})$ / kcal mol^{-1}	Zero point energy ZPE / kcal mol^{-1}
Thergas[37]	**26.96**[a]	
PM3	13.59	56.718
PM3 UHF	3.25	56.081
AM1	15.39	58.405
AM1 UHF	4.72	59.027

[a]Benson's method.

	Moments of inertia of the molecule / g cm$^2 \times 10^{-39}$		
MOPAC method	I_a	I_b	I_c
PM3	**15.388 94**	**29.83852**	**45.2213**
PM3 UHF	15.394 39	30.0644	45.4588
AM1	15.299 83	30.18327	45.4830
AM1 UHF	15.318 16	30.38217	45.7003

	Molecular vibrations / cm^{-1}					
PM3	**122**	**338**	**421**	**473**	**509**	**597**
	608	**782**	**794**	**877**	**914**	**963**
	974	**1002**	**1094**	**1103**	**1141**	**1157**
	1217	**1285**	**1406**	**1410**	**1658**	**1682**
	1864	**3048**	**3052**	**3060**	**3068**	**3075**
PM3 UHF	133	314	407	469	510	589
	595	749	765	861	872	922
	952	966	1085	1089	1144	1148
	1214	1400	1401	1409	1593	1596
	1760	3050	3052	3065	3069	3077
AM1	142	351	430	479	541	619
	635	815	833	931	947	980
	1002	1039	1146	1169	1205	1212
	1297	1356	1455	1473	1672	1692
	1952	3175	3176	3186	3187	3196
AM1 UHF	146	329	418	476	539	602
	630	783	803	905	924	936
	958	1034	1145	1156	1202	1207
	1297	1449	1461	1476	1609	1617
	1829	3179	3179	3189	3191	3198

TABLE 32. Thermodynamic properties of $\cdot C_6H_5O$ (2,4-cyclohexadiene-1-one-2-yl radical) (M_r=93.105)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	C_p° (J·K^{-1}·mol^{-1})	$H°-H°(T_r)$ (J·mol^{-1})	$S°$ (J·K^{-1}·mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}·mol^{-1})	$H(T)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	log K_f
0	—	−16.926	—	—	95.875	127.706	—
100	42.964	−13.239	252.362	384.751	99.562	122.077	−68.5570
200	65.958	−7.891	288.522	327.976	104.910	117.272	−37.1673
298.15	95.207	0.000	320.233	320.233	112.801	112.801	−27.2545
300	95.768	0.177	320.824	320.235	112.977	112.722	−27.1326
400	124.520	11.222	352.400	324.346	124.022	108.878	−22.3046
500	148.726	24.925	382.878	333.027	137.726	105.785	−19.5001
600	168.285	40.811	411.787	343.769	153.612	103.304	−17.6791
700	184.108	58.458	438.958	355.447	171.258	101.344	−16.4064
800	197.083	77.538	464.417	367.495	190.339	99.845	−15.4683
900	207.867	97.802	488.272	379.603	210.602	98.763	−14.7479
1000	216.922	119.054	510.655	391.601	231.855	98.030	−14.1768
1100	224.583	141.140	531.699	403.390	253.940	97.599	−13.7125
1200	231.104	163.933	551.528	414.917	276.733	97.415	−13.3266
1300	236.681	187.329	570.252	426.152	300.130	97.429	−13.0008
1400	241.474	211.243	587.971	437.084	324.043	97.585	−12.7206
1500	245.611	235.602	604.776	447.708	348.403	97.864	−12.4780
1600	249.198	260.347	620.745	458.028	373.147	98.222	−12.2648
1700	252.321	285.426	635.948	468.050	398.227	98.630	−12.0757
1800	255.052	310.798	650.449	477.784	423.599	99.071	−11.9069
1900	257.449	336.425	664.305	487.239	449.226	99.523	−11.7553
2000	259.563	362.278	677.565	496.426	475.079	99.974	−11.6180
2100	261.433	388.330	690.275	505.356	501.131	100.410	−11.4935
2200	263.095	414.558	702.476	514.041	527.359	100.812	−11.3797
2300	264.576	440.943	714.205	522.490	553.743	101.186	−11.2755
2400	265.902	467.468	725.493	530.715	580.269	101.515	−11.1798
2500	267.091	494.119	736.373	538.725	606.919	101.784	−11.0910
2600	268.163	520.882	746.869	546.530	633.683	102.009	−11.0091
2700	269.131	547.748	757.008	554.139	660.548	102.168	−10.9333
2800	270.008	574.705	766.812	561.560	687.506	102.264	−10.8628
2900	270.804	601.747	776.301	568.802	714.547	102.292	−10.7968
3000	271.530	628.864	785.494	575.873	741.664	102.237	−10.7351
3100	272.192	656.050	794.409	582.779	768.851	102.128	−10.6781
3200	272.798	683.300	803.060	589.529	796.101	101.931	−10.6243
3300	273.355	710.608	811.463	596.127	823.409	101.659	−10.5739
3400	273.866	737.970	819.631	602.581	850.770	101.309	−10.5266
3500	274.338	765.380	827.577	608.897	878.181	100.869	−10.4824
3600	274.773	792.836	835.311	615.079	905.637	100.355	−10.4405
3700	275.176	820.334	842.846	621.134	933.135	99.749	−10.4014
3800	275.549	847.870	850.189	627.065	960.671	99.059	−10.3643
3900	275.895	875.443	857.351	632.879	988.243	98.285	−10.3297
4000	276.217	903.049	864.340	638.578	1015.849	97.409	−10.2967
4100	276.517	930.686	871.164	644.168	1043.486	96.460	−10.2661
4200	276.797	958.351	877.831	649.652	1071.152	95.414	−10.2370
4300	277.059	986.044	884.348	655.035	1098.845	94.271	−10.2093
4400	277.304	1013.763	890.720	660.319	1126.563	93.018	−10.1832
4500	277.533	1041.505	896.954	665.509	1154.305	91.690	−10.1589
4600	277.748	1069.269	903.056	670.607	1182.069	90.274	−10.1359
4700	277.950	1097.054	909.032	675.616	1209.854	88.772	−10.1143
4800	278.140	1124.858	914.886	680.540	1237.659	87.182	−10.0941
4900	278.319	1152.681	920.623	685.382	1265.482	85.503	−10.0751
5000	278.488	1180.522	926.247	690.143	1293.322	83.677	−10.0567
5100	278.647	1208.379	931.764	694.827	1321.179	81.831	−10.0403
5200	278.797	1236.251	937.176	699.435	1349.051	79.860	−10.0243
5300	278.939	1264.138	942.488	703.971	1376.938	77.798	−10.0094
5400	279.074	1292.038	947.703	708.437	1404.839	75.647	−9.9954
5500	279.202	1319.952	952.825	712.834	1432.753	73.408	−9.9823
5600	279.323	1347.879	957.857	717.164	1460.679	71.080	−9.9700
5700	279.437	1375.817	962.802	721.430	1488.617	68.668	−9.9586
5800	279.547	1403.766	967.663	725.634	1516.566	66.170	−9.9480
5900	279.650	1431.726	972.442	729.777	1544.526	63.590	−9.9380
6000	279.749	1459.696	977.143	733.861	1572.496	60.931	−9.9288

TABLE 33. Molecular properties of $C_{12}H_4OCl_4$ (2,3,6,7-tetrachlorodibenzofuran). Values listed with bold characters were chosen for thermodynamic calculations—$\sigma = \mathbf{1}$ and statistical weight = **1**

		Enthalpy of formation $\Delta_f H°(298.15\ \mathrm{K})$/kcal mol^{-1}			Zero point energy ZPE / kcal mol^{-1}	
Dorofeeva[39]		**−11.95±2.4**				
PM3		2.966			79.879	
		Moments of inertia of the molecule / g cm^2×10^{-39}				
MOPAC method		I_a		I_b		I_c
PM3		94.526 089		601.764 87		696.290 96
Dorofeeva[48]		**96.411 819**		**613.417 36**		**709.829 18**
		Molecular vibrations / cm^{-1}				
Dorofeeva[48]	**53**	**58**	**118**	**126**	**168**	**173**
B3LYP	**186**	**218**	**234**	**260**	**282**	**330**
	369	**392**	**407**	**442**	**473**	**506**
	565	**577**	**629**	**654**	**676**	**685**
	709	**732**	**760**	**777**	**796**	**822**
	836	**903**	**926**	**948**	**975**	**981**
	1036	**1099**	**1125**	**1215**	**1232**	**1244**
	1262	**1311**	**1330**	**1379**	**1412**	**1473**
	1488	**1551**	**1584**	**1595**	**1623**	**3051**
	3052(3)					
PM3	44.7	53.9	98	110.9	152	165.3
	178	195.5	234	268	276	316
	340	384	401	417	447	480
	496	598	606	611	667	677
	710	726	767	792	857	918
	926	932	947	953	985	1075
	1116	1141	1155	1164	1285	1331
	1341	1378	1442	1509	1528	1578
	1616	1758	1794	1819	1842	3055
	3069	3074	3078			

TABLE 34. Thermodynamic properties of $C_{12}H_4OCl_4$ (2,3,6,7-tetrachlorodibenzofuran) (M_r=305.974)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	C_p° (J·K^{-1}·mol^{-1})	$H°-H°(T_r)$ (J·mol^{-1})	$S°$ (J·K^{-1}·mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}·mol^{-1})	$H(T)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	log K_f
0	—	−38.205	—	—	−88.205	−35.924	—
100	96.293	−32.166	331.342	653.002	−82.166	−43.895	4.8518
200	163.634	−19.132	419.015	514.675	−69.132	−47.704	−7.0444
298.15	225.108	0.000	496.028	496.028	−50.000	−50.000	−11.2396
300	226.193	0.417	497.423	496.032	−49.583	−50.032	−11.2936
400	279.472	25.792	570.053	505.574	−24.208	−51.175	−13.4973
500	321.731	55.941	637.154	525.272	5.941	−51.463	−14.8391
600	354.346	89.816	698.825	549.131	39.816	−51.219	−15.7333
700	379.538	126.563	755.421	574.616	76.563	−50.588	−16.3669
800	399.251	165.541	807.440	600.513	115.541	−49.639	−16.8350
900	414.922	206.279	855.404	626.205	156.279	−48.408	−17.1909
1000	427.566	248.425	899.798	651.372	198.425	−46.963	−17.4679
1100	437.900	291.715	941.050	675.854	241.715	−45.337	−17.6873
1200	446.442	335.946	979.530	699.575	285.946	−43.574	−17.8632
1300	453.571	380.957	1015.554	722.510	330.957	−41.719	−18.0067
1400	459.572	426.622	1049.393	744.663	376.622	−39.836	−18.1231
1500	464.664	472.841	1081.279	766.051	422.841	−37.913	−18.2206
1600	469.014	519.531	1111.410	786.703	469.531	−36.010	−18.3013
1700	472.755	566.624	1139.959	806.651	516.624	−34.153	−18.3686
1800	475.992	614.065	1167.074	825.927	564.065	−32.353	−18.4254
1900	478.809	661.808	1192.887	844.567	611.808	−30.631	−18.4735
2000	481.272	709.815	1217.511	862.603	659.815	−28.998	−18.5139
2100	483.438	758.053	1241.046	880.068	708.053	−27.467	−18.5494
2200	485.351	806.494	1263.580	896.992	756.494	−26.071	−18.5795
2300	487.047	855.116	1285.193	913.404	805.116	−24.793	−18.6058
2400	488.558	903.897	1305.954	929.330	853.897	−23.659	−18.6292
2500	489.909	952.822	1325.926	944.797	902.822	−22.699	−18.6489
2600	491.122	1001.875	1345.165	959.828	951.875	−21.882	−18.6667
2700	492.213	1051.042	1363.721	974.446	1001.042	−21.250	−18.6830
2800	493.199	1100.314	1381.639	988.670	1050.314	−20.800	−18.6978
2900	494.093	1149.679	1398.962	1002.521	1099.679	−20.537	−18.7106
3000	494.905	1199.130	1415.727	1016.017	1149.130	−20.495	−18.7225
3100	495.645	1248.658	1431.967	1029.174	1198.658	−20.621	−18.7346
3200	496.321	1298.256	1447.714	1042.009	1248.256	−20.970	−18.7456
3300	496.940	1347.920	1462.996	1054.535	1297.920	−21.524	−18.7559
3400	497.508	1397.643	1477.840	1066.768	1347.643	−22.284	−18.7659
3500	498.031	1447.420	1492.269	1078.720	1397.420	−23.268	−18.7763
3600	498.513	1497.248	1506.306	1090.404	1447.248	−24.439	−18.7859
3700	498.959	1547.122	1519.971	1101.830	1497.122	−25.827	−18.7960
3800	499.371	1597.038	1533.282	1113.009	1547.038	−27.412	−18.8055
3900	499.754	1646.995	1546.259	1123.953	1596.995	−29.186	−18.8158
4000	500.109	1696.988	1558.916	1134.669	1646.988	−31.173	−18.8255
4100	500.440	1747.016	1571.269	1145.168	1697.016	−33.312	−18.8362
4200	500.748	1797.075	1583.332	1155.457	1747.075	−35.641	−18.8468
4300	501.036	1847.165	1595.119	1165.545	1797.165	−38.151	−18.8570
4400	501.305	1897.282	1606.640	1175.440	1847.282	−40.855	−18.8673
4500	501.557	1947.425	1617.909	1185.148	1897.425	−43.679	−18.8786
4600	501.793	1997.593	1628.935	1194.676	1947.593	−46.640	−18.8899
4700	502.015	2047.783	1639.729	1204.031	1997.783	−49.727	−18.9015
4800	502.223	2097.995	1650.301	1213.218	2047.995	−52.934	−18.9139
4900	502.420	2148.228	1660.658	1222.244	2098.228	−56.256	−18.9263
5000	502.604	2198.479	1670.810	1231.114	2148.479	−59.805	−18.9380
5100	502.779	2248.748	1680.765	1239.834	2198.748	−63.315	−18.9516
5200	502.943	2299.034	1690.529	1248.407	2249.034	−67.005	−18.9643
5300	503.099	2349.337	1700.111	1256.840	2299.337	−70.790	−18.9773
5400	503.246	2399.654	1709.516	1265.136	2349.654	−74.668	−18.9907
5500	503.386	2449.986	1718.752	1273.300	2399.986	−78.633	−19.0042
5600	503.518	2500.331	1727.823	1281.336	2450.331	−82.681	−19.0178
5700	503.644	2550.689	1736.737	1289.247	2500.689	−86.808	−19.0318
5800	503.763	2601.059	1745.497	1297.038	2551.059	−91.012	−19.0458
5900	503.876	2651.441	1754.109	1304.712	2601.441	−95.289	−19.0599
6000	503.984	2701.834	1762.579	1312.273	2651.834	−99.630	−19.0743

TABLE 35. Molecular properties of $C_{12}H_4OCl_4$ (2,4,6,8-tetrachlorodibenzofuran). Values listed with bold characters were chosen for thermodynamic calculations—$\sigma = \mathbf{2}$ and statistical weight $= \mathbf{1}$

	Enthalpy of formation $\Delta_f H°(298.15\ \mathrm{K})$/kcal mol^{-1}	Zero point energy ZPE / kcal mol^{-1}
Dorofeeva[39]	**−13.86±2.4**	
PM3	6.55	79.505

Moments of inertia of the molecule / g cm^2×10^{-39}

	I_a	I_b	I_c
PM3	189.010	437.992	627.003
Dorofeeva[48]	197.908 94	445.592 24	643.501 187

Molecular vibrations / cm^{-1}

Dorofeeva[48]	**39**	**78**	**105**	**145**	**166**	**170**
B3LYP	**191**	**209**	**219**	**231**	**315**	**363**
	367	**386**	**392**	**401**	**401**	**547**
	568	**568**	**574**	**640**	**683**	**701**
	742	**768**	**769**	**815**	**825**	**851**
	879	**884**	**890**	**910**	**952**	**967**
	1000	**1086**	**1129**	**1214**	**1244**	**1254**
	1265	**1309**	**1333**	**1378**	**1404**	**1474**
	1489	**1542**	**1582**	**1588**	**1624**	**3050**
	3051	**3053**	**3053**			
PM3	62.1	82.1	107.7	140.1	153.7	165.1
	185.6	199	211	238	306	334
	357	368	373	380	393	498
	561	570	576	605	624	657
	721	737	757	785	895	904
	942	949	949	957	971	1074
	1095	1153	1167	1173	1303	1340
	1349	1351	1407	1503	1564	1581
	1621	1761	1771	1810	1818	3005
	3005	3024	3026			

TABLE 36. Thermodynamic properties of $C_{12}H_4OCl_4$ (2,4,6,8-tetrachlorodibenzofuran) (M_r=305.974)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	C_p° (J·K^{-1}·mol^{-1})	$H°-H°(T_r)$ (J·mol^{-1})	$S°$ (J·K^{-1}·mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}·mol^{-1})	$H(T)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	log K_f
0	—	−38.388	—	—	−96.388	−44.108	—
100	97.070	−32.328	327.606	650.882	−90.328	−52.057	8.9197
200	164.506	−19.194	415.968	511.936	−77.194	−55.766	−5.0982
298.15	225.552	0.000	493.238	493.238	−58.000	−58.000	−9.9838
300	226.633	0.418	494.636	493.242	−57.582	−58.031	−10.0464
400	279.769	25.828	567.369	502.799	−32.172	−59.139	−12.5976
500	321.974	56.004	634.529	522.521	−1.996	−59.400	−14.1470
600	354.554	89.901	696.241	546.406	31.901	−59.133	−15.1792
700	379.717	126.668	752.867	571.913	68.668	−58.483	−15.9111
800	399.405	165.663	804.909	597.830	107.663	−57.518	−16.4528
900	415.054	206.415	852.889	623.540	148.415	−56.272	−16.8659
1000	427.680	248.573	897.296	648.723	190.573	−54.815	−17.1884
1100	438.000	291.874	938.558	673.218	233.874	−53.178	−17.4451
1200	446.529	336.114	977.047	696.952	278.114	−51.406	−17.6520
1300	453.648	381.133	1013.077	719.898	323.133	−49.543	−17.8217
1400	459.640	426.806	1046.922	742.061	368.806	−47.652	−17.9605
1500	464.724	473.031	1078.812	763.458	415.031	−45.723	−18.0774
1600	469.068	519.726	1108.947	784.118	461.726	−43.815	−18.1752
1700	472.803	566.824	1137.499	804.073	508.824	−41.952	−18.2574
1800	476.036	614.270	1164.617	823.356	556.270	−40.148	−18.3276
1900	478.848	662.017	1190.432	842.002	604.017	−38.422	−18.3875
2000	481.308	710.028	1215.058	860.044	652.028	−36.785	−18.4387
2100	483.471	758.269	1238.594	877.514	700.269	−35.251	−18.4839
2200	485.381	806.714	1261.130	894.442	748.714	−33.851	−18.5227
2300	487.075	855.338	1282.744	910.858	797.338	−32.571	−18.5571
2400	488.584	904.123	1303.507	926.789	846.123	−31.433	−18.5879
2500	489.933	953.050	1323.479	942.260	895.050	−30.471	−18.6143
2600	491.144	1002.105	1342.719	957.294	944.105	−29.652	−18.6383
2700	492.234	1051.274	1361.276	971.915	993.274	−29.018	−18.6604
2800	493.219	1100.548	1379.195	986.142	1042.548	−28.566	−18.6806
2900	494.111	1149.915	1396.519	999.996	1091.915	−28.301	−18.6984
3000	494.922	1199.367	1413.284	1013.495	1141.367	−28.257	−18.7150
3100	495.661	1248.897	1429.524	1026.654	1190.897	−28.382	−18.7314
3200	496.336	1298.497	1445.272	1039.491	1240.497	−28.729	−18.7465
3300	496.954	1348.162	1460.554	1052.020	1290.162	−29.282	−18.7607
3400	497.521	1397.886	1475.398	1064.255	1339.886	−30.041	−18.7743
3500	498.044	1447.665	1489.828	1076.209	1389.665	−31.023	−18.7881
3600	498.525	1497.494	1503.865	1087.895	1439.494	−32.193	−18.8009
3700	498.970	1547.369	1517.530	1099.323	1489.369	−33.580	−18.8140
3800	499.382	1597.287	1530.843	1110.504	1539.287	−35.164	−18.8264
3900	499.764	1647.244	1543.819	1121.449	1589.244	−36.937	−18.8394
4000	500.119	1697.239	1556.477	1132.167	1639.239	−38.922	−18.8517
4100	500.449	1747.267	1568.830	1142.667	1689.267	−41.061	−18.8649
4200	500.757	1797.328	1580.893	1152.958	1739.328	−43.389	−18.8779
4300	501.044	1847.418	1592.680	1163.048	1789.418	−45.898	−18.8903
4400	501.313	1897.536	1604.202	1172.944	1839.536	−48.601	−18.9027
4500	501.565	1947.680	1615.471	1182.653	1889.680	−51.424	−18.9161
4600	501.800	1997.848	1626.497	1192.182	1939.848	−54.385	−18.9293
4700	502.022	2048.040	1637.291	1201.538	1990.040	−57.471	−18.9428
4800	502.230	2098.252	1647.863	1210.727	2040.252	−60.678	−18.9569
4900	502.426	2148.485	1658.220	1219.754	2090.485	−63.998	−18.9710
5000	502.611	2198.737	1668.373	1228.625	2140.737	−67.547	−18.9845
5100	502.785	2249.007	1678.327	1237.346	2191.007	−71.056	−18.9996
5200	502.949	2299.294	1688.092	1245.920	2241.294	−74.746	−19.0139
5300	503.105	2349.596	1697.674	1254.354	2291.596	−78.530	−19.0284
5400	503.252	2399.914	1707.079	1262.651	2341.914	−82.408	−19.0432
5500	503.391	2450.246	1716.315	1270.816	2392.246	−86.372	−19.0580
5600	503.523	2500.592	1725.386	1278.852	2442.592	−90.420	−19.0729
5700	503.648	2550.951	1734.300	1286.764	2492.951	−94.546	−19.0881
5800	503.767	2601.322	1743.060	1294.556	2543.322	−98.750	−19.1034
5900	503.881	2651.704	1751.673	1302.231	2593.704	−103.026	−19.1187
6000	503.988	2702.098	1760.142	1309.793	2644.098	−107.367	−19.1342

TABLE 37. Molecular properties of $C_{12}H_4O_2Cl_4$ (2,3,7,8-tetrachlorodibenzo-*p*-dioxin). Values listed with bold characters were chosen for thermodynamic calculations—$\sigma = \mathbf{4}$ and statistical weight = **1**

	Enthalpy of formation $\Delta_f H°(298.15\ \text{K})$ / kcal mol^{-1}	Zero point energy ZPE / kcal mol^{-1}
Dorofeeva[39]	**−39.197±3.6**	
PM3	−32.27	82.384

Moments of inertia of the molecule / g cm^2×10^{-39}

MOPAC Method	I_a	I_b	I_c
PM3	**96.390 84**	**752.119 56**	**847.418 35**

Molecular vibrations / cm^{-1}

PM3	26.9	44.6	96.3	116.5	130.6	159.9
	168.2	169.2	194	229	247	262
	319	377	382	392	418	425
	440	478	525	616	622	654
	662	672	696	698	703	804
	860	931	933	942	944	945
	974	984	1127	1128	1186	1188
	1312	1313	1329	1334	1422	1430
	1524	1556	1595	1637	1757	1762
	1792	1799	3050	3051	3051	3052
PM3[a]	19.30	44.54	97.59	118.6	129.4	162.5
	168	178	197	231	244	262
	320	378	379	387	422	428
	443	475	528	619	622	652
	661	672	696	700	703	807
	863	927	929	939	940	942
	972	989	1122	1123	1184	1185
	1310	1323	1335	1339	1423	1424
	1535	1569	1595	1636	1732	1733
	1798	1799	3060	3061	3062	3062
B3LYP/6-31G**[b]	**20.07**	**49.43**	**113**	**114**	**138**	**173**
	185	**200**	**222**	**230**	**258**	**286**
	328	**382**	**392**	**393**	**448**	**451**
	459	**499**	**542**	**559**	**625**	**625**
	645	**652**	**665**	**668**	**693**	**763**
	794	**851**	**852**	**884**	**885**	**900**
	938	**992**	**1132**	**1135**	**1188**	**1192**
	1244	**1261**	**1269**	**1320**	**1346**	**1349**
	1401	**1427**	**1519**	**1531**	**1613**	**1629**
	1648	**1683**	**3235**	**3235**	**3236**	**3236**

[a]Values calculated by Ruben Asatryan from Armenian Institute of Chemical Physics, The Armenian Academy of Sciences, Yerevan, Armenia.
[b]B.J. Mhin, J. Choi, and W. Choi, ''A simple rule for classification of polychlorinated dibenzo-*p*-dioxin congeners,'' J. Am. Chem. Soc. **123**, 3584 (2001); supporting information.

TABLE 38. Thermodynamic properties of $C_{12}H_4O_2Cl_4$ (2,3,7,8-tetrachlorodibenzo-*p*-dioxin) (M_r=321.973)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	C_p° (J·K^{-1}·mol^{-1})	$H°-H°(T_r)$ (J·mol^{-1})	$S°$ (J·K^{-1}·mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}·mol^{-1})	$H(T)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	log K_f
0	—	−41.226	—	—	−205.226	−148.606	—
100	103.161	−34.717	335.305	682.475	−198.717	−157.556	59.9017
200	177.304	−20.636	429.954	533.134	−184.636	−161.774	18.2650
298.15	241.524	0.000	513.049	513.049	−164.000	−164.000	4.2636
300	242.635	0.448	514.547	513.054	−163.552	−164.029	4.0864
400	296.857	27.519	592.051	523.254	−136.481	−164.961	−3.0755
500	339.814	59.442	663.106	544.223	−104.558	−165.005	−7.3860
600	373.072	95.158	728.132	569.536	−68.842	−164.499	−10.2550
700	398.827	133.806	787.658	596.506	−30.194	−163.595	−12.2958
800	419.019	174.738	842.285	623.863	10.738	−162.362	−13.8167
900	435.105	217.474	892.602	650.964	53.474	−160.835	−14.9894
1000	448.118	261.657	939.142	677.485	97.657	−159.085	−15.9180
1100	458.789	307.020	982.369	703.260	143.020	−157.142	−16.6691
1200	467.641	353.354	1022.680	728.218	189.354	−155.049	−17.2868
1300	475.055	400.500	1060.412	752.335	236.500	−152.853	−17.8030
1400	481.320	448.327	1095.853	775.620	284.327	−150.615	−18.2378
1500	486.654	496.733	1129.248	798.092	332.733	−148.326	−18.6104
1600	491.226	545.633	1160.805	819.785	381.633	−146.049	−18.9311
1700	495.170	594.957	1190.707	840.732	430.957	−143.807	−19.2093
1800	498.592	644.649	1219.109	860.971	480.649	−141.616	−19.4530
1900	501.578	694.661	1246.148	880.537	530.661	−139.497	−19.6676
2000	504.195	744.953	1271.944	899.468	580.953	−137.462	−19.8574
2100	506.501	795.490	1296.601	917.796	631.490	−135.527	−20.0275
2200	508.542	846.244	1320.211	935.555	682.244	−133.724	−20.1796
2300	510.355	897.191	1342.857	952.775	733.191	−132.040	−20.3168
2400	511.972	948.308	1364.613	969.484	784.308	−130.498	−20.4415
2500	513.420	999.579	1385.542	985.711	835.579	−129.133	−20.5540
2600	514.722	1050.988	1405.705	1001.479	886.988	−127.912	−20.6572
2700	515.895	1102.519	1425.153	1016.813	938.519	−126.879	−20.7523
2800	516.956	1154.163	1443.934	1031.733	990.163	−126.030	−20.8399
2900	517.918	1205.907	1462.092	1046.262	1041.907	−125.372	−20.9203
3000	518.793	1257.744	1479.665	1060.418	1093.744	−124.938	−20.9950
3100	519.591	1309.663	1496.690	1074.218	1145.663	−124.677	−21.0657
3200	520.321	1361.659	1513.198	1087.679	1197.659	−124.643	−21.1314
3300	520.990	1413.726	1529.219	1100.818	1249.726	−124.818	−21.1928
3400	521.604	1465.856	1544.782	1113.648	1301.856	−125.203	−21.2509
3500	522.170	1518.045	1559.910	1126.183	1354.045	−125.816	−21.3063
3600	522.692	1570.288	1574.627	1138.436	1406.288	−126.621	−21.3584
3700	523.175	1622.582	1588.955	1150.420	1458.582	−127.648	−21.4085
3800	523.622	1674.922	1602.913	1162.144	1510.922	−128.876	−21.4557
3900	524.036	1727.305	1616.520	1173.621	1563.305	−130.297	−21.5017
4000	524.422	1779.728	1629.793	1184.860	1615.728	−131.935	−21.5452
4100	524.780	1832.189	1642.746	1195.871	1668.189	−133.731	−21.5880
4200	525.115	1884.684	1655.396	1206.662	1720.684	−135.720	−21.6290
4300	525.427	1937.211	1667.756	1217.242	1773.211	−137.895	−21.6680
4400	525.720	1989.768	1679.839	1227.619	1825.768	−140.269	−21.7059
4500	525.993	2042.354	1691.656	1237.800	1878.354	−142.767	−21.7433
4600	526.250	2094.966	1703.220	1247.793	1930.966	−145.406	−21.7795
4700	526.491	2147.604	1714.540	1257.603	1983.604	−148.175	−21.8150
4800	526.718	2200.264	1725.627	1267.239	2036.264	−151.069	−21.8501
4900	526.931	2252.947	1736.490	1276.705	2088.947	−154.082	−21.8843
5000	527.132	2305.650	1747.137	1286.007	2141.650	−157.326	−21.9169
5100	527.322	2358.373	1757.578	1295.152	2194.373	−160.535	−21.9504
5200	527.501	2411.114	1767.819	1304.143	2247.114	−163.929	−21.9822
5300	527.670	2463.872	1777.869	1312.987	2299.872	−167.420	−22.0136
5400	527.831	2516.648	1787.734	1321.688	2352.648	−171.009	−22.0446
5500	527.982	2569.438	1797.420	1330.250	2405.438	−174.688	−22.0750
5600	528.126	2622.244	1806.935	1338.677	2458.244	−178.454	−22.1049
5700	528.263	2675.063	1816.284	1346.974	2511.063	−182.303	−22.1344
5800	528.393	2727.896	1825.472	1355.145	2563.896	−186.232	−22.1636
5900	528.516	2780.742	1834.506	1363.194	2616.742	−190.236	−22.1922
6000	528.634	2833.599	1843.390	1371.123	2669.599	−194.308	−22.2206

TABLE 39. Molecular properties of $C_{12}H_4O_2Cl_4$ (1,3,6,8-tetrachlorodibenzo-*p*-dioxin). Values listed with bold characters were chosen for thermodynamic calculations—$\sigma = \mathbf{2}$ and statistical weight = **1**

	Enthalpy of formation $\Delta_f H°$(298.15 K) / kcal mol^{-1}	Zero point energy ZPE / kcal mol^{-1}
Dorofeeva[39]	**−41.35±3.6**	
PM3	−31.74	82.406

Moments of inertia of the molecule / g cm^2×10^{-39}

MOPAC method	I_a	I_b	I_c
PM3	**177.084 39**	**530.216 25**	**707.208 77**

Molecular vibrations / cm^{-1}

PM3	24.4	44.5	106.7	112.9	148.7	150.5
	155.2	193.8	197	199	212	300
	339	352	361	396	398	452
	493	535	538	553	565	567
	622	709	724	726	735	810
	886	912	922	923	940	942
	978	1028	1103	1108	1171	1178
	1310	1329	1335	1337	1412	1413
	1544	1574	1596	1633	1758	1764
	1793	1800	3057	3057	3062	3062
B3LYP/6-31G**[a]	**20.12**	**48.35**	**105**	**128**	**155**	**156**
	158	**198**	**203**	**223**	**249**	**298**
	350	**357**	**372**	**402**	**410**	**463**
	486	**535**	**537**	**564**	**576**	**576**
	590	**668**	**682**	**703**	**703**	**827**
	851	**852**	**858**	**865**	**867**	**868**
	963	**989**	**1111**	**1112**	**1193**	**1218**
	1235	**1245**	**1267**	**1326**	**1338**	**1355**
	1441	**1457**	**1509**	**1513**	**1618**	**1619**
	1651	**1669**	**3240**	**3240**	**3246**	**3246**
Dorofeeva[48]	28	50	104	124	151	156
B3LYP/	161	210	213	214	233	290
	357	359	364	388	390	465
	466	533	549	555	567	592
	633	706	709	761	771	781
	818	825	881	881	904	905
	944	959	1008	1030	1130	1213
	1232	1253	1281	1302	1339	1357
	1383	1399	1481	1484	1567	1578
	1584	1634	3051	3051	3053	3053

[a]B. J. Mhin, J. Choi, and W. Choi, ''A simple rule for classification of polychlorinated dibenzo-*p*-dioxin congeners,'' J. Am. Chem. Soc. **123**, 3584 (2001); supporting information.

TABLE 40. Thermodynamic properties of $C_{12}H_4O_2Cl_4$ (1,3,6,8-tetrachlorodibenzo-*p*-dioxin) (M_r=321.973)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	C_p° (J·K^{-1}·mol^{-1})	$H°-H°(T_r)$ (J·mol^{-1})	$S°$ (J·K^{-1}·mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}·mol^{-1})	$H(T)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	log K_f
0	—	−41.467	—	—	−214.467	−157.847	—
100	104.644	−34.882	342.565	691.387	−207.882	−166.722	65.0682
200	178.101	−20.683	438.059	541.476	−193.683	−170.821	21.0512
298.15	241.759	0.000	521.354	521.354	−173.000	−173.000	6.2741
300	242.864	0.448	522.853	521.359	−172.552	−173.028	6.0872
400	296.860	27.529	600.386	531.564	−145.471	−173.951	−1.4661
500	339.741	59.447	671.433	552.538	−113.553	−173.999	−6.0115
600	372.977	95.155	736.443	577.852	−77.845	−173.502	−9.0371
700	398.725	133.794	795.954	604.820	−39.206	−172.608	−11.1900
800	418.916	174.715	850.567	632.173	1.715	−171.385	−12.7950
900	435.003	217.441	900.872	659.271	44.441	−169.869	−14.0332
1000	448.019	261.614	947.401	685.787	88.614	−168.129	−15.0142
1100	458.693	306.967	990.619	711.558	133.967	−166.195	−15.8083
1200	467.549	353.292	1030.922	736.511	180.292	−164.112	−16.4619
1300	474.967	400.429	1068.647	760.625	227.429	−161.925	−17.0083
1400	481.237	448.247	1104.082	783.905	275.247	−159.695	−17.4693
1500	486.575	496.645	1137.470	806.374	323.645	−157.415	−17.8645
1600	491.151	545.537	1169.023	828.062	372.537	−155.145	−18.2049
1700	495.100	594.854	1198.920	849.006	421.854	−152.910	−18.5006
1800	498.526	644.539	1227.319	869.241	471.539	−150.726	−18.7598
1900	501.516	694.545	1254.354	888.804	521.545	−148.613	−18.9884
2000	504.137	744.830	1280.147	907.732	571.830	−146.584	−19.1907
2100	506.447	795.362	1304.801	926.057	622.362	−144.655	−19.3722
2200	508.491	846.111	1328.409	943.813	673.111	−142.857	−19.5345
2300	510.307	897.053	1351.053	961.030	724.053	−141.178	−19.6812
2400	511.927	948.166	1372.806	977.737	775.166	−139.641	−19.8146
2500	513.378	999.432	1393.734	993.961	826.432	−138.280	−19.9350
2600	514.682	1050.836	1413.895	1009.727	877.836	−137.063	−20.0456
2700	515.857	1102.364	1433.342	1025.059	929.364	−136.034	−20.1474
2800	516.920	1154.004	1452.122	1039.977	981.004	−135.189	−20.2414
2900	517.884	1205.745	1470.278	1054.504	1032.745	−134.534	−20.3277
3000	518.761	1257.578	1487.850	1068.658	1084.578	−134.104	−20.4079
3100	519.561	1309.495	1504.874	1082.456	1136.495	−133.845	−20.4837
3200	520.292	1361.488	1521.381	1095.916	1188.488	−133.814	−20.5542
3300	520.963	1413.551	1537.401	1109.053	1240.551	−133.992	−20.6202
3400	521.579	1465.679	1552.963	1121.881	1292.679	−134.380	−20.6825
3500	522.146	1517.865	1568.091	1134.415	1344.865	−134.996	−20.7420
3600	522.669	1570.106	1582.807	1146.667	1397.106	−135.803	−20.7979
3700	523.152	1622.398	1597.135	1158.649	1449.398	−136.832	−20.8516
3800	523.600	1674.736	1611.092	1170.372	1501.736	−138.062	−20.9023
3900	524.016	1727.117	1624.698	1181.848	1554.117	−139.485	−20.9514
4000	524.402	1779.538	1637.970	1193.086	1606.538	−141.126	−20.9980
4100	524.762	1831.996	1650.924	1204.095	1658.996	−142.924	−21.0437
4200	525.097	1884.489	1663.573	1214.885	1711.489	−144.914	−21.0875
4300	525.410	1937.015	1675.933	1225.464	1764.015	−147.091	−21.1292
4400	525.703	1989.571	1688.015	1235.840	1816.571	−149.467	−21.1696
4500	525.977	2042.155	1699.832	1246.020	1869.155	−151.966	−21.2095
4600	526.235	2094.765	1711.395	1256.012	1921.765	−154.607	−21.2480
4700	526.476	2147.401	1722.715	1265.821	1974.401	−157.378	−21.2857
4800	526.704	2200.060	1733.802	1275.456	2027.060	−160.273	−21.3230
4900	526.917	2252.741	1744.664	1284.921	2079.741	−163.287	−21.3592
5000	527.119	2305.443	1755.311	1294.223	2132.443	−166.533	−21.3937
5100	527.309	2358.165	1765.752	1303.366	2185.165	−169.743	−21.4291
5200	527.489	2410.905	1775.993	1312.357	2237.905	−173.138	−21.4628
5300	527.659	2463.662	1786.042	1321.200	2290.662	−176.630	−21.4959
5400	527.819	2516.436	1795.907	1329.900	2343.436	−180.220	−21.5286
5500	527.972	2569.226	1805.593	1338.461	2396.226	−183.901	−21.5606
5600	528.116	2622.030	1815.108	1346.888	2449.030	−187.668	−21.5921
5700	528.253	2674.849	1824.456	1355.185	2501.849	−191.517	−21.6231
5800	528.383	2727.681	1833.645	1363.355	2554.681	−195.448	−21.6537
5900	528.507	2780.525	1842.678	1371.403	2607.525	−199.452	−21.6837
6000	528.625	2833.382	1851.562	1379.332	2660.382	−203.525	−21.7135

TABLE 41. Molecular properties of $C_{12}H_4Cl_4O_3$ (1,3,6,8-tetrachlorodibenzo-*p*-dioxin-2-ol). Values listed with bold characters were chosen for thermodynamic calculations—$\sigma = \mathbf{1}$ and statistical weight = **1**

	Enthalpy of formation $\Delta_f H°(298.15\ \mathrm{K})$ / kcal mol^{-1}	Zero point energy ZPE / kcal mol^{-1}
Our estimate	**−70.59**	
PM3	−74.98	85.823
PM3 UHF	−75.859	84.835
AM1	−56.53	88.876
AM1 UHF	−58.73	

Moments of inertia of the molecule / g cm$^2 \times 10^{-39}$

MOPAC method	I_a	I_b	I_c
PM3	**183.064 92**	**587.555 52**	**770.615 73**
PM3 UHF	183.268 23	588.431 75	717.699 23
AM1	183.065 43	587.554 20	770.612 63
AM1 UHF	186.668 46	592.787 26	778.213 07

Reduced moment of inertia[34] $I_r(\mathrm{OH}) = \mathbf{0.136\ 43}$ g cm$^2 \times 10^{-39}$; $\sigma_{\mathrm{rot}} = \mathbf{2}$; $V(2) = \mathbf{1116.8}$ cm^{-1}.

Molecular vibrations / cm^{-1}

PM3	20.6	**41.9**	**92.9**	**106.3**	**112.4**	**149.2**
	158.4	**169**	**198**	**203**	**203**	**274**
	289	**299**	**314**	**343**	**362**	**378**
	401	**403**	**452**	**514**	**527**	**535**
	565	**587**	**626**	**661**	**690**	**725**
	729	**768**	**800**	**839**	**902**	**922**
	932	**940**	**957**	**1033**	**1105**	**1114**
	1174	**1241**	**1289**	**1326**	**1330**	**1337**
	1404	**1426**	**1512**	**1555**	**1598**	**1611**
	1637	**1761**	**1766**	**1795**	**1800**	**3057**
	3058	**3062**	**3855**			
PM3 UHF	23.64	40.7	88.3	106	108	146
	158	166	197	197	202	272
	281	298	314	332	360	376
	386	401	449	507	511	518
	547	585	626	630	686	699
	722	729	795	833	893	900
	903	916	951	1018	1097	1105
	1172	1232	1318	1334	1342	1361
	1386	1451	1474	1533	1572	1582
	1603	1695	1700	1729	1735	3059
	3060	3064	3857			
AM1	23.61	41.34	86.9	90	133	156
	173	185	210	217	219	246
	303	325	344	360	400	420
	426	457	497	544	550	559
	579	622	660	678	710	735
	748	826	900	933	939	941
	943	978	1060	1137	1199	1209
	1262	1332	1356	1393	1410	1432
	1481	1498	1585	1600	1650	1665
	1694	1745	1757	1787	1794	3174
	3183	3188	3402			
AM1 UHF	18.07	37.5	80.36	95.7	122	146
	167	176	195	216	217	272
	287	321	340	344	395	399
	422	452	493	519	528	547
	553	615	620	667	677	691
	737	819	890	906	908	912
	933	966	1052	1129	1190	1202
	1262	1325	1382	1424	1431	1441
	1453	1514	1561	1573	1630	1634
	1655	1674	1693	1714	1730	3175
	3184	3191	3404			

TABLE 42. Thermodynamic properties of $C_{12}H_4Cl_4O_3$ (1,3,6,8-tetrachlorodibenzo-*p*-dioxin-2-ol) (M_r=337.973)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	C_p° ($J\cdot K^{-1}\cdot mol^{-1}$)	$H°-H°(T_r)$ ($J\cdot mol^{-1}$)	$S°$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$-[G°-H°(T_r)]/T$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$H(T)$ ($kJ\cdot mol^{-1}$)	$\Delta_f H°$ ($kJ\cdot mol^{-1}$)	log K_f
0	—	−43.948	—	—	−339.318	−278.357	—
100	110.331	−37.467	341.390	716.061	−332.837	−288.787	124.2394
200	192.455	−22.155	444.253	555.026	−317.525	−293.229	48.2902
298.15	256.811	0.000	533.525	533.525	−295.370	−295.370	22.9901
300	257.903	0.476	535.117	533.530	−294.894	−295.398	22.6712
400	311.017	29.017	616.859	544.315	−266.353	−296.345	9.7913
500	353.410	62.322	690.999	566.356	−233.048	−296.537	2.0478
600	386.776	99.398	758.505	592.841	−195.972	−296.251	−3.1130
700	413.022	139.440	820.178	620.978	−155.930	−295.581	−6.7938
800	433.846	181.822	876.741	649.463	−113.548	−294.566	−9.5468
900	450.570	226.073	928.841	677.649	−69.297	−293.228	−11.6792
1000	464.170	271.833	977.041	705.208	−23.537	−291.633	−13.3767
1100	475.359	318.827	1021.823	731.980	23.457	−289.814	−14.7574
1200	484.660	366.842	1063.595	757.894	71.472	−287.816	−15.9004
1300	492.462	415.709	1102.706	782.930	120.339	−285.691	−16.8611
1400	499.062	465.294	1139.449	807.097	169.924	−283.502	−17.6773
1500	504.686	515.489	1174.078	830.419	220.119	−281.246	−18.3805
1600	509.511	566.205	1206.808	852.930	270.835	−278.988	−18.9904
1700	513.677	617.369	1237.825	874.666	321.999	−276.753	−19.5240
1800	517.293	668.922	1267.290	895.667	373.552	−274.561	−19.9946
1900	520.450	720.812	1295.345	915.970	425.442	−272.435	−20.4123
2000	523.220	772.999	1322.113	935.613	477.629	−270.387	−20.7848
2100	525.661	825.445	1347.701	954.632	530.075	−268.438	−21.1202
2200	527.823	878.122	1372.206	973.060	582.752	−266.619	−21.4225
2300	529.744	931.002	1395.712	990.928	635.632	−264.920	−21.6969
2400	531.459	984.064	1418.294	1008.268	688.694	−263.363	−21.9474
2500	532.996	1037.288	1440.021	1025.106	741.918	−261.986	−22.1756
2600	534.377	1090.658	1460.953	1041.469	795.288	−260.755	−22.3855
2700	535.622	1144.159	1481.144	1057.382	848.789	−259.715	−22.5794
2800	536.749	1197.778	1500.644	1072.866	902.408	−258.864	−22.7588
2900	537.771	1251.505	1519.498	1087.944	956.135	−258.208	−22.9246
3000	538.701	1305.329	1537.745	1102.635	1009.959	−257.780	−23.0791
3100	539.550	1359.243	1555.423	1116.958	1063.873	−257.529	−23.2244
3200	540.326	1413.237	1572.565	1130.929	1117.867	−257.511	−23.3600
3300	541.038	1467.306	1589.203	1144.565	1171.936	−257.707	−23.4872
3400	541.691	1521.443	1605.365	1157.881	1226.073	−258.118	−23.6071
3500	542.293	1575.642	1621.076	1170.892	1280.272	−258.762	−23.7209
3600	542.849	1629.900	1636.360	1183.611	1334.530	−259.602	−23.8281
3700	543.363	1684.211	1651.241	1196.049	1388.841	−260.670	−23.9304
3800	543.838	1738.571	1665.738	1208.219	1443.201	−261.943	−24.0270
3900	544.280	1792.977	1679.870	1220.133	1497.607	−263.416	−24.1199
4000	544.691	1847.426	1693.655	1231.799	1552.056	−265.110	−24.2080
4100	545.073	1901.914	1707.110	1243.229	1606.544	−266.967	−24.2932
4200	545.429	1956.440	1720.249	1254.430	1661.070	−269.021	−24.3746
4300	545.762	2010.999	1733.087	1265.413	1715.629	−271.267	−24.4522
4400	546.074	2065.591	1745.638	1276.185	1770.221	−273.716	−24.5269
4500	546.365	2120.214	1757.913	1286.754	1824.844	−276.294	−24.5996
4600	546.639	2174.864	1769.925	1297.128	1879.494	−279.018	−24.6695
4700	546.896	2229.541	1781.683	1307.313	1934.171	−281.877	−24.7373
4800	547.138	2284.243	1793.200	1317.316	1988.873	−284.864	−24.8033
4900	547.365	2338.968	1804.484	1327.144	2043.598	−287.976	−24.8672
5000	547.580	2393.715	1815.544	1336.801	2098.345	−291.322	−24.9283
5100	547.782	2448.483	1826.390	1346.295	2153.113	−294.639	−24.9893
5200	547.973	2503.271	1837.029	1355.630	2207.901	−298.144	−25.0476
5300	548.154	2558.078	1874.468	1364.812	2262.708	−301.750	−25.1044
5400	548.325	2612.902	1857.716	1373.845	2317.532	−305.460	−25.1600
5500	548.487	2667.742	1867.779	1382.735	2372.372	−309.262	−25.2140
5600	548.641	2722.599	1877.663	1391.485	2427.229	−313.156	−25.2667
5700	548.786	2777.470	1887.375	1400.100	2482.100	−317.135	−25.3183
5800	548.925	2832.356	1896.921	1408.584	2536.986	−321.199	−25.3688
5900	549.057	2887.255	1906.305	1416.940	2591.855	−325.340	−25.4180
6000	549.182	2942.167	1915.535	1425.173	2646.797	−329.553	−25.4663

TABLE 43. Molecular properties of $C_{12}H_4Cl_5O_2\cdot$ (2,4-dichlorophenoxy-1′,3′,5′-trichlorophenyl-6-6′-ether radical–$Cl_2C_6H_2(O\cdot)$–O–$C_6H_2Cl_3$). Values listed with bold characters were chosen for thermodynamic calculations—$\sigma = \mathbf{1}$ and statistical weight = **2**

	Enthalpy of formation $\Delta_f H°(298.15\ \mathrm{K})$ / kcal mol^{-1}	Zero point energy ZPE / kcal mol^{-1}
Our estimate	**−30.62±6.0**	
NIST 94[17]	−33.7	
PM3	−17.41	81.110
PM3 UHF	−29.34	80.336
AM1	−9.88	85.293
AM1 UHF	−21.17	84.307

Moments of inertia of the molecule / g cm$^2\times10^{-39}$

MOPAC method	I_a	I_b	I_c
PM3	**212.474 12**	**647.327 722**	**661.920 80**
PM3 UHF	216.561 95	655.924 756	676.466 06
AM1	218.107 15	660.782 78	679.722 27
AM1 UHF	218.872 27	661.159 82	680.536 54

Reduced moment of inertia[34] I_r(tch) = **84.513** 93 g cm$^2\times10^{-39}$; $\sigma_{rot} = \mathbf{2}$; $V(2) = \mathbf{1116}$ cm^{-1}.
I_r(dcp) = **74.007** g cm$^2\times10^{-39}$; $\sigma_{rot} = \mathbf{2}$; $V(2) = \mathbf{1116}$ cm^{-1}.

Molecular vibrations / cm^{-1}

PM3	12.4	19.8	**30.5**	**57.7**	**81.2**	**129**
	143	**149**	**169**	**185**	**186**	**194**
	220	**263**	**310**	**323**	**338**	**365**
	370	**389**	**423**	**449**	**481**	**518**
	530	**541**	**553**	**571**	**643**	**716**
	755	**766**	**787**	**812**	**871**	**897**
	924	**924**	**937**	**946**	**962**	**1079**
	1090	**1156**	**1162**	**1191**	**1263**	**1308**
	1315	**1385**	**1414**	**1448**	**1517**	**1571**
	1626	**1673**	**1754**	**1766**	**1874**	**3042**
	3048	**3056**	**3059**			
PM3 UHF	13.9	16.2	31	50.4	77.9	126
	140	148	160	179	185	193
	215	266	282	331	334	365
	370	401	422	435	469	508
	520	523	544	561	623	720
	743	745	788	805	862	871
	885	902	911	931	969	1075
	1090	1156	1163	1172	1283	1348
	1356	1390	1420	1450	1496	1553
	1569	1602	1710	1723	1802	3042
	3051	3055	3058			
AM1	14.7	18.14	33.7	51.3	79.5	133
	147	158	175	186	199	207
	235	302	304	355	359	406
	439	448	464	473	515	555
	557	564	586	593	656	771
	775	853	908	915	921	942
	944	947	960	981	1082	1188
	1207	1253	1257	1302	1240	1357
	1392	1469	1473	1503	1540	1622
	1672	1704	1732	1746	1977	3163
	3171	3174	3174			
AM1 UHF	11.8	16.5	30.1	50.9	78.1	129
	145	154	299	351	356	398
	436	447	461	469	483	523
	539	550	581	583	649	750
	756	847	878	901	902	913
	922	924	953	972	1075	1182
	1202	1256	1261	1293	1377	1413
	1442	1458	1485	1510	1518	1589
	1613	1656	1675	1689	1869	3166
	3173	3175	3177			

TABLE 44. Thermodynamic properties of $C_{12}H_4Cl_5O_2$· (2,4-dichlorophenoxy-1′,3′,5′-trichlorophenyl-6-2′-ether radical) (M_r=357.426)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	C_p° (J·K^{-1}·mol^{-1})	$H°-H°(T_r)$ (J·mol^{-1})	$S°$ (J·K^{-1}·mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}·mol^{-1})	$H(T)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	log K_f
0	—	−48.225	—	—	−176.339	−115.128	—
100	128.751	−39.849	403.112	801.600	−167.963	−123.668	40.8060
200	203.682	−23.099	516.231	631.726	−151.213	−126.736	8.1370
298.15	265.216	0.000	609.381	609.381	−128.114	−128.114	−2.8178
300	266.271	0.492	611.025	609.386	−127.622	−128.131	−2.9561
400	317.361	29.770	694.901	620.476	−98.344	−128.590	−8.5448
500	357.479	63.596	770.216	643.023	−64.518	−128.516	−11.9033
600	388.602	100.966	838.263	669.986	−27.148	−128.173	−14.1380
700	412.893	141.090	900.065	698.509	12.976	−127.630	−15.7290
800	432.104	183.376	956.502	727.282	55.262	−126.892	−16.9166
900	447.518	227.384	1008.319	755.670	99.270	−125.953	−17.8339
1000	460.047	272.783	1056.140	783.357	144.669	−124.856	−18.5619
1100	470.346	319.319	1100.486	810.195	191.205	−123.614	−19.1520
1200	478.897	366.795	1141.789	836.127	238.680	−122.263	−19.6385
1300	486.057	415.053	1180.412	861.141	286.938	−120.840	−20.0461
1400	492.101	463.969	1216.661	885.254	335.855	−119.405	−20.3902
1500	497.239	513.443	1250.792	908.497	385.329	−117.944	−20.6862
1600	501.636	563.392	1283.027	930.907	435.278	−116.517	−20.9416
1700	505.423	613.750	1313.555	952.526	485.635	−115.146	−21.1640
1800	508.703	664.460	1342.539	973.395	536.346	−113.848	−21.3595
1900	511.559	715.476	1370.121	993.555	587.362	−112.639	−21.5324
2000	514.060	766.760	1396.426	1013.046	638.646	−111.532	−21.6859
2100	516.259	818.278	1421.561	1031.905	690.164	−110.543	−21.8243
2200	518.202	870.003	1445.624	1050.168	741.889	−109.703	−21.9486
2300	519.927	921.911	1468.697	1067.866	793.797	−109.000	−22.0616
2400	521.464	973.982	1490.858	1085.032	845.868	−108.457	−22.1650
2500	522.838	1026.198	1512.174	1101.695	898.084	−108.110	−22.2587
2600	524.071	1078.545	1532.704	1117.879	950.431	−107.926	−22.3454
2700	525.182	1131.009	1552.504	1133.612	1002.895	−107.950	−22.4260
2800	526.186	1183.578	1571.622	1148.916	1055.464	−108.179	−22.5009
2900	527.096	1236.243	1590.103	1163.812	1108.129	−108.621	−22.5702
3000	527.923	1288.994	1607.987	1178.322	1160.880	−109.309	−22.6352
3100	528.676	1341.825	1625.309	1192.463	1213.711	−110.192	−22.6973
3200	529.365	1394.727	1642.105	1206.253	1266.613	−111.325	−22.7557
3300	529.996	1447.696	1658.405	1219.709	1319.582	−112.689	−22.8109
3400	530.575	1500.725	1674.235	1232.846	1372.611	−114.285	−22.8635
3500	531.108	1553.809	1689.623	1245.678	1425.695	−116.130	−22.9145
3600	531.599	1606.945	1704.592	1258.218	1478.831	−118.187	−22.9628
3700	532.053	1660.128	1719.163	1270.480	1532.014	−120.485	−23.0098
3800	532.473	1713.354	1733.358	1282.475	1585.240	−123.001	−23.0547
3900	532.863	1766.621	1747.194	1294.214	1638.507	−125.727	−23.0987
4000	533.225	1819.926	1760.690	1305.708	1691.812	−128.683	−23.1410
4100	533.563	1873.266	1773.861	1316.967	1745.152	−131.808	−23.1829
4200	533.877	1926.638	1786.722	1327.999	1798.524	−135.137	−23.2235
4300	534.170	1980.040	1799.288	1338.813	1851.926	−138.660	−23.2626
4400	534.445	2033.471	1811.571	1349.419	1905.357	−142.387	−23.3009
4500	534.702	2086.929	1823.585	1359.823	1958.815	−146.241	−23.3391
4600	534.942	2140.411	1835.340	1370.033	2012.297	−150.238	−23.3763
4700	535.169	2193.917	1846.847	1380.056	2065.803	−154.364	−23.4131
4800	535.381	2247.444	1858.116	1389.899	2119.330	−158.612	−23.4498
4900	535.581	2300.992	1869.157	1399.567	2172.878	−162.974	−23.4858
5000	535.770	2354.560	1879.979	1409.067	2226.446	−167.562	−23.5204
5100	535.948	2408.146	1890.591	1418.405	2280.032	−172.106	−23.5561
5200	536.115	2461.749	1901.000	1427.586	2333.635	−176.824	−23.5904
5300	536.274	2515.369	1911.213	1436.615	2387.255	−181.630	−23.6243
5400	536.424	2569.004	1921.239	1445.497	2440.890	−186.521	−23.6581
5500	536.567	2622.653	1931.083	1454.237	2494.539	−191.489	−23.6913
5600	536.702	2676.317	1940.752	1462.839	2548.203	−196.529	−23.7242
5700	536.830	2729.994	1950.253	1471.307	2601.879	−201.636	−23.7568
5800	536.951	2783.683	1959.590	1479.645	2655.569	−206.807	−23.7890
5900	537.067	2837.384	1968.770	1487.858	2709.270	−212.036	−23.8209
6000	537.177	2891.096	1977.798	1495.948	2762.982	−217.316	−23.8526

TABLE 45. Molecular properties of $C_{12}H_4O_2Cl_6$ (2,4,6-trichlorocyclohexa-3,5-diene-1-one-1′,3′,5′-trichlorophenyl-2-6′-ether). Values listed with bold characters were chosen for thermodynamic calculations—$\sigma = \mathbf{1}$ and statistical weight = **1**

	Enthalpy of formation $\Delta_f H°(298.15\ \text{K})$ / kcal mol^{-1}	Zero point energy ZPE / kcal mol^{-1}
Our estimate	**−35.0**	
PM3	−35.162	82.722
PM3 UHF	−35.386	81.422
AM1	−23.83	87.095

Moments of inertia of the molecule / g cm^2 × 10^{-39}

MOPAC method	I_a	I_b	I_c
PM3	**246.485 89**	**629.756**	**762.771 37**
PM3 UHF	259.718 63	615.0278	719.029 85
AM1	251.858 9	633.5244	740.994 86

Reduced moment of inertia[34] I_r(tcp) = **72.5050** g cm^2 × 10^{-39}; $\sigma_{rot} = \mathbf{2}$; $V(2) = \mathbf{1116}$ cm^{-1}.
I_r(tcp-o-) = **133.1776** g cm^2 × 10^{-39}; $\sigma_{rot} = \mathbf{2}$; $V(2) = \mathbf{1116}$ cm^{-1}.

Molecular vibrations / cm^{-1}

PM3	8.74	17.1	**34.15**	**50.6**	**102**	**114**
	131	**142**	**147**	**149**	**183**	**187**
	193	**198**	**220**	**282**	**324**	**338**
	354	**370**	**372**	**405**	**405**	**424**
	434	**516**	**531**	**545**	**552**	**570**
	621	**666**	**716**	**740**	**787**	**790**
	798	**850**	**903**	**919**	**924**	**941**
	947	**987**	**1077**	**1085**	**1139**	**1158**
	1177	**1205**	**1300**	**1308**	**1333**	**1383**
	1417	**1512**	**1574**	**1749**	**1767**	**1828**
	1842	**1973**	**3040**	**3044**	**3055**	**3059**
PM3 UHF	8.52	21.87	32.93	50.9	86.5	113
	129	141	148	152	182	184
	194	199	217	286	320	337
	349	362	370	397	402	423
	432	505	520	521	549	558
	626	660	711	736	781	785
	792	844	874	898	910	911
	931	967	1074	1083	1139	1157
	1167	1187	1301	1307	1349	1354
	1414	1447	1493	1555	1693	1708
	1724	1958	3042	3045	3056	3059
AM1	10.4	27.78	32.13	53.67	83.5	117
	136	146	155	161	188	195
	202	218	234	311	349	358
	393	402	437	438	455	465
	470	555	560	571	592	595
	655	722	769	826	852	901
	913	927	945	947	952	957
	983	1070	1176	1197	1235	1261
	1282	1318	1371	1379	1401	1457
	1476	1537	1627	1728	1745	1821
	1832	2064	3160	3166	3171	3174

TABLE 46. Thermodynamic properties of $C_{12}H_4O_2Cl_6$ (2,4,6-trichlorocyclohexa-3,5-diene-one-1′,3′,5′-trichlorophenyl-2-6′-ether) (M_r= 392.879)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	C_p° (J·K^{-1}·mol^{-1})	$H°-H°(T_r)$ (J·mol^{-1})	$S°$ (J·K^{-1}·mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}·mol^{-1})	$H(T)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	log K_f
0	—	−51.665	—	—	−198.105	−132.303	—
100	138.230	−42.900	406.423	835.422	−189.340	−141.910	45.5713
200	219.548	−24.856	528.256	652.537	−171.296	−145.203	8.1046
298.15	284.786	0.000	628.505	628.505	−146.440	−146.440	−4.4344
300	285.891	0.528	630.270	628.511	−145.912	−146.452	−4.5925
400	338.827	31.873	720.079	640.397	−114.567	−146.580	−10.9726
500	379.767	67.892	800.284	664.500	−78.548	−146.098	−14.7962
600	411.306	107.513	872.434	693.246	−38.927	−145.320	−17.3335
700	435.872	149.922	937.758	723.585	3.482	−144.328	−19.1350
800	455.307	194.517	997.279	754.132	48.077	−143.131	−20.4763
900	470.915	240.856	1051.840	784.222	94.416	−141.722	−21.5099
1000	483.617	288.604	1102.135	813.532	142.164	−140.144	−22.3281
1100	494.069	337.504	1148.735	841.913	191.064	−138.414	−22.9896
1200	502.753	387.359	1192.108	869.309	240.919	−136.564	−23.5338
1300	510.030	438.008	1232.646	895.716	291.568	−134.636	−23.9884
1400	516.175	489.327	1270.674	921.155	342.887	−132.690	−24.3714
1500	521.401	541.213	1306.469	945.661	394.773	−130.712	−24.6998
1600	525.875	593.582	1340.266	969.277	447.142	−128.766	−24.9824
1700	529.728	646.367	1372.266	992.050	499.927	−126.873	−25.2278
1800	533.066	699.511	1402.641	1014.024	553.071	−125.051	−25.4429
1900	535.974	752.966	1431.542	1035.244	606.526	−123.318	−25.6325
2000	538.519	806.693	1459.100	1055.753	660.253	−121.688	−25.8004
2100	540.758	860.660	1485.430	1075.592	714.220	−120.177	−25.9511
2200	542.737	914.836	1510.632	1094.798	768.396	−118.819	−26.0860
2300	544.493	969.200	1534.798	1113.406	822.760	−117.604	−26.2081
2400	546.058	1023.729	1558.005	1131.451	877.289	−116.555	−26.3194
2500	547.457	1078.406	1580.325	1148.963	931.966	−115.710	−26.4200
2600	548.713	1133.215	1601.821	1165.969	986.775	−115.039	−26.5126
2700	549.844	1188.144	1622.551	1182.498	1041.704	−114.586	−26.5983
2800	550.867	1243.180	1642.567	1198.574	1096.740	−114.353	−26.6776
2900	551.793	1298.314	1661.914	1214.219	1151.874	−114.346	−26.7508
3000	552.635	1353.536	1680.635	1229.456	1207.096	−114.600	−26.8191
3100	553.403	1408.839	1698.768	1244.304	1262.399	−115.067	−26.8841
3200	554.104	1464.215	1716.349	1258.782	1317.775	−115.799	−26.9449
3300	554.746	1519.657	1733.410	1272.908	1373.217	−116.780	−27.0022
3400	555.336	1575.162	1749.980	1286.697	1428.722	−118.010	−27.0566
3500	555.879	1630.723	1766.086	1300.165	1484.283	−119.506	−27.1092
3600	556.379	1686.336	1781.752	1313.326	1539.896	−121.230	−27.1588
3700	556.842	1741.998	1797.003	1326.193	1595.558	−123.210	−27.2070
3800	557.270	1797.704	1811.859	1338.779	1651.264	−125.422	−27.2528
3900	557.667	1853.451	1826.339	1351.095	1707.011	−127.855	−27.2976
4000	558.036	1909.236	1840.463	1363.154	1762.796	−130.530	−27.3405
4100	558.379	1965.057	1854.246	1374.964	1818.617	−133.384	−27.3830
4200	558.699	2020.911	1867.706	1386.537	1874.471	−136.447	−27.4241
4300	558.998	2076.796	1880.856	1397.880	1930.356	−139.711	−27.4635
4400	559.277	2132.710	1893.710	1409.003	1986.270	−143.180	−27.5020
4500	559.539	2188.651	1906.282	1419.915	2042.211	−146.779	−27.5404
4600	559.784	2244.617	1918.583	1430.622	2098.177	−150.521	−27.5777
4700	560.015	2300.607	1930.624	1441.133	2154.167	−154.388	−27.6146
4800	560.231	2356.620	1942.416	1451.454	2210.180	−158.372	−27.6512
4900	560.435	2412.653	1953.970	1461.592	2266.213	−162.464	−27.6872
5000	560.627	2468.706	1965.294	1471.553	2322.266	−166.773	−27.7216
5100	560.808	2524.778	1976.398	1481.343	2378.338	−171.029	−27.7572
5200	560.979	2580.868	1987.290	1490.969	2434.428	−175.449	−27.7912
5300	561.141	2636.974	1997.977	1500.434	2490.534	−179.943	−27.8248
5400	561.294	2693.095	2008.467	1509.746	2546.655	−184.510	−27.8582
5500	561.439	2749.232	2018.768	1518.907	2602.792	−189.138	−27.8911
5600	561.576	2805.383	2028.885	1527.924	2658.943	−193.822	−27.9235
5700	561.706	2861.547	2038.826	1536.800	2715.107	−198.557	−27.9557
5800	561.830	2917.724	2048.596	1545.540	2771.284	−203.339	−27.9874
5900	561.948	2973.913	2058.201	1554.148	2827.473	−208.161	−28.0187
6000	562.060	3030.113	2067.647	1562.628	2883.673	−213.016	−28.0498

TABLE 47. Molecular properties of $C_6HCl_3OH-C_6HCl_3OH$ (2,4,6,2′,4′,6′-hexachloro-biphenyl-3,3′-diol). Values listed with bold characters were chosen for thermodynamic calculations—$\sigma = \mathbf{2}$ and statistical weight = **1**

	Enthalpy of formation $\Delta_f H°(298.15\ \text{K})$ / kcal mol^{-1}			Zero point energy ZPE / kcal mol^{-1}	
THERM[37]	**−76.94±8**				
PM3	−69.063			84.847	
	Moments of inertia of the molecule / g cm^2×10^{-39}				
MOPAC method	I_a	I_b		I_c	
PM3	**225.756 74**	**649.180 09**		**662.572 04**	

Reduced moment of inertia[34] (I_r(OH) = **0.142 48** g cm^2×10^{-39}; $\sigma_{rot} = \mathbf{2}$; $V(2) = \mathbf{1116}$ cm^{-1})×2.
I_r(tcp-tcp) = **66.590** g cm^2×10^{-39}; $\sigma_{rot} = \mathbf{2}$; $V(2) = \mathbf{1116}$ cm^{-1}.

Molecular vibrations / cm^{-1}

PM3	43.0	45.8	46.6	**90.8**	**93.3**	**105.7**
	106.3	**138.7**	**167**	**168**	**188**	**195**
	198	**234**	**300**	**303**	**326**	**327**
	358	**358**	**370**	**378**	**392**	**413**
	455	**539**	**543**	**561**	**596**	**609**
	612	**628**	**694**	**700**	**726**	**730**
	773	**802**	**814**	**818**	**905**	**953**
	955	**1081**	**1125**	**1167**	**1182**	**1227**
	1263	**1265**	**1382**	**1418**	**1431**	**1484**
	1539	**1563**	**1566**	**1657**	**1732**	**1737**
	1751	**1776**	**3003**	**3005**	**3617**	**3622**

TABLE 48. Thermodynamic properties of $C_{12}H_4Cl_6O_2$ (2,4,6,2′,4′,6′-hexachloro-biphenyl-3,3′-diol) (M_r=392.879)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	C_p° (J·K^{-1}·mol^{-1})	$H°-H°(T_r)$ (J·mol^{-1})	$S°$ (J·K^{-1}·mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}·mol^{-1})	$H(T)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	log K_f
0	—	−49.483	—	—	−371.400	−305.599	—
100	124.498	−42.236	357.115	779.480	−364.153	−316.724	134.3067
200	217.649	−24.905	473.526	598.053	−346.822	−320.729	51.0875
298.15	286.707	0.000	573.925	573.925	−321.917	−321.917	23.4567
300	287.837	0.531	575.702	573.931	−321.386	−321.925	23.1090
400	341.147	32.102	666.156	585.902	−289.815	−321.828	9.0953
500	381.782	68.339	746.850	610.171	−253.578	−321.128	0.6975
600	412.894	108.141	819.331	639.096	−213.776	−320.169	−4.8856
700	436.986	150.685	884.865	669.601	−171.232	−319.041	−8.8609
800	455.944	195.368	944.503	700.293	−126.549	−317.757	−11.8314
900	471.119	241.748	999.113	730.504	−80.169	−316.306	−14.1316
1000	483.454	289.497	1049.411	759.913	−32.420	−314.727	−15.9630
1100	493.618	338.367	1095.980	788.374	16.450	−313.028	−17.4536
1200	502.086	388.164	1139.305	815.834	66.248	−311.235	−18.6888
1300	509.211	438.739	1179.782	842.291	116.822	−309.382	−19.7284
1400	515.254	489.971	1217.746	867.767	168.054	−307.523	−20.6130
1500	520.418	541.761	1253.476	892.302	219.844	−305.641	−21.3764
1600	524.860	594.030	1287.208	915.939	272.113	−303.795	−22.0398
1700	528.704	646.713	1319.145	938.726	324.796	−302.004	−22.6215
1800	532.049	699.754	1349.462	960.710	377.837	−300.284	−23.1356
1900	534.974	753.109	1378.309	981.936	431.192	−298.652	−23.5929
2000	537.545	806.737	1405.816	1002.447	484.820	−297.121	−24.0018
2100	539.815	860.608	1432.099	1022.286	538.691	−295.706	−24.3708
2200	541.827	914.692	1457.259	1041.490	592.775	−294.441	−24.7042
2300	543.618	968.966	1481.384	1060.095	647.049	−293.314	−25.0077
2400	545.219	1023.409	1504.555	1078.134	701.492	−292.351	−25.2853
2500	546.654	1078.004	1526.841	1095.640	756.087	−291.589	−25.5389
2600	547.945	1132.735	1548.307	1112.640	810.818	−290.996	−25.7729
2700	549.111	1187.589	1569.009	1129.161	865.672	−290.618	−25.9895
2800	550.166	1242.553	1588.998	1145.229	920.636	−290.457	−26.1905
2900	551.124	1297.619	1608.321	1160.866	975.702	−290.518	−26.3770
3000	551.996	1352.775	1627.020	1176.095	1030.858	−290.838	−26.5511
3100	552.792	1408.015	1645.133	1190.934	1086.098	−291.367	−26.7151
3200	553.521	1463.331	1662.695	1205.404	1141.414	−292.159	−26.8688
3300	554.189	1518.717	1679.738	1219.521	1196.800	−293.197	−27.0133
3400	554.803	1574.167	1696.292	1233.301	1252.250	−294.482	−27.1499
3500	555.369	1629.676	1712.382	1246.760	1307.759	−296.030	−27.2799
3600	555.891	1685.240	1728.035	1259.913	1363.323	−297.804	−27.4027
3700	556.374	1740.853	1743.272	1272.772	1418.936	−299.831	−27.5201
3800	556.822	1796.513	1758.116	1285.349	1474.596	−302.089	−27.6315
3900	557.238	1852.217	1772.585	1297.658	1530.300	−304.566	−27.7387
4000	557.624	1907.960	1786.698	1309.708	1586.043	−307.283	−27.8407
4100	557.984	1963.741	1800.472	1321.511	1641.824	−310.177	−27.9395
4200	558.320	2019.556	1813.922	1333.075	1697.639	−313.279	−28.0343
4300	558.633	2075.404	1827.063	1344.411	1753.487	−316.580	−28.1248
4400	558.927	2131.282	1839.909	1355.527	1809.365	−320.085	−28.2121
4500	559.202	2187.189	1852.473	1366.431	1865.272	−323.718	−28.2972
4600	559.460	2243.122	1864.767	1377.131	1921.205	−327.493	−28.3792
4700	559.702	2299.080	1876.801	1387.635	1977.163	−331.392	−28.4588
4800	559.930	2355.062	1888.587	1397.949	2033.145	−335.407	−28.5364
4900	560.144	2411.066	1900.135	1408.080	2089.149	−339.528	−28.6117
5000	560.347	2467.090	1911.453	1418.035	2145.173	−343.866	−28.6839
5100	560.537	2523.134	1922.551	1427.819	2201.217	−348.150	−28.7557
5200	560.718	2579.197	1933.438	1437.438	2257.280	−352.597	−28.8246
5300	560.888	2635.278	1944.120	1446.898	2313.361	−357.116	−28.8918
5400	561.050	2691.375	1954.606	1456.203	2369.458	−361.708	−28.9576
5500	561.202	2747.487	1964.902	1465.359	2425.570	−366.360	−29.0216
5600	561.347	2803.615	1975.015	1474.370	2481.698	−371.067	−29.0841
5700	561.485	2859.757	1984.952	1483.240	2537.840	−375.824	−29.1452
5800	561.616	2915.912	1994.718	1491.975	2593.995	−380.628	−29.2050
5900	561.740	2972.080	2004.320	1500.578	2650.163	−385.472	−29.2633
6000	561.859	3028.260	2013.762	1509.052	2706.343	−390.346	−29.3206

TABLE 49. Molecular properties of $C_{12}H_5Cl_3O_3$ (2,4,7-trichlorodibenzo-*p*-dioxin-9-ol). Values listed with bold characters were chosen for thermodynamic calculations—$\sigma = \mathbf{1}$ and statistical weight $= \mathbf{1}$

	Enthalpy of formation $\Delta_f H°(298.15\ \mathrm{K})$ / kcal mol^{-1}	Zero point energy ZPE / kcal mol^{-1}
Our estimate	**−83.41**	
PM3	−68.426	91.952
PM3 UHF	−69.807	90.692
AM1	−54.027	94.760
AM1 UHF	−55.929	93.581

Moments of inertia of the molecule / g cm$^2 \times 10^{-39}$

MOPAC method	I_a	I_b	I_c
PM3	**139.999 55**	**516.769 12**	**656.574 45**
PM3 UHF	138.939 77	514.993 31	653.645 19
AM1	141.604 69	515.358 44	653.790 19
AM1 UHF	141.025 94	518.897 17	658.931 97

Reduced moment of inertia[36] $I_r(\mathrm{OH}) = \mathbf{0.1425}$ g cm$^2 \times 10^{-39}$; $\sigma_{\mathrm{rot}} = \mathbf{2}$; $V(2) = \mathbf{1116}$ cm^{-1}.

Molecular vibrations / cm^{-1}

PM3	30.7	**53.9**	**113.1**	**119.3**	**154.2**	**172**
	173	**195**	**205**	**205**	**257**	**271**
	302	**344**	**356**	**368**	**392**	**463**
	501	**531**	**533**	**563**	**567**	**569**
	580	**621**	**713**	**721**	**732**	**763**
	854	**898**	**908**	**921**	**926**	**933**
	945	**1003**	**1109**	**1144**	**1169**	**1202**
	1277	**1311**	**1344**	**1353**	**1385**	**1412**
	1448	**1485**	**1552**	**1597**	**1629**	**1663**
	1763	**1770**	**1802**	**1811**	**3040**	**3041**
	3053	**3129**	**3880**			
PM3 UHF	24.05	51.2	105	118	149	167
	177	200	208	211	257	292
	301	331	344	371	399	461
	487	517	530	542	550	553
	577	624	689	703	712	765
	850	882	898	902	906	918
	919	994	1098	1106	1162	1180
	1213	1305	1332	1350	1361	1401
	1440	1443	1537	1566	1592	1616
	1703	1705	1739	1742	3057	3058
	3063	3067	3884			
AM1	22.84	48.7	99	132	155	175
	186	205	217	223	260	267
	336	354	367	412	455	508
	522	553	567	575	580	584
	613	680	694	711	775	859
	914	930	937	940	963	975
	1019	1108	1200	1207	1249	1267
	1307	1362	1394	1423	1444	1487
	1512	1554	1592	1641	1678	1722
	1751	1759	1803	1805	3175	3189
	3189	3195	3443			
AM1 UHF	21.67	46.4	101.5	125	148	166
	185	196	208	222	257	265
	332	337	348	408	451	505
	517	529	544	554	558	565
	606	654	669	678	766	851
	887	903	908	912	954	964
	1013	1100	1191	1199	1243	1267
	1306	1394	1426	1433	1446	1473
	1517	1535	1566	1616	1646	1682
	1685	1694	1739	1743	3177	3189
	3190	3195	3443			

TABLE 50. Thermodynamic properties of $C_{12}H_5Cl_3O_3$ (2,4,7-trichlorodibenzo-*p*-dioxin-9-ol) (M_r=303.528)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	C_p° (J·K^{-1}·mol^{-1})	$H°-H°(T_r)$ (J·mol^{-1})	$S°$ (J·K^{-1}·mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}·mol^{-1})	$H(T)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	log K_f
0	—	−40.642	—	—	−389.630	−329.026	—
100	100.498	−34.721	327.444	674.656	−383.709	−340.059	152.5975
200	177.974	−20.663	421.802	525.118	−369.651	−345.583	63.1556
298.15	241.279	0.000	505.020	505.020	−348.987	−348.987	33.3078
300	242.370	0.447	506.516	505.025	−348.540	−349.039	32.9308
400	295.959	27.452	583.834	515.204	−321.536	−351.241	17.6910
500	339.343	59.298	654.716	536.120	−289.690	−352.567	8.4998
600	373.829	95.023	719.756	561.383	−253.964	−353.281	2.3551
700	401.198	133.827	779.517	588.336	−215.161	−353.482	−2.0401
800	423.099	175.081	834.572	615.721	−173.906	−353.222	−5.3367
900	440.833	218.308	885.465	642.901	−130.679	−352.534	−7.8969
1000	455.363	263.141	932.688	669.547	−85.846	−351.499	−9.9402
1100	467.397	309.298	976.671	695.492	−39.690	−350.162	−11.6063
1200	477.459	356.555	1017.784	720.655	7.568	−348.579	−12.9889
1300	485.941	404.737	1056.346	745.010	55.749	−346.813	−14.1537
1400	493.146	453.701	1092.629	768.557	104.713	−344.937	−15.1457
1500	499.308	503.331	1126.868	791.313	154.344	−342.953	−16.0021
1600	504.609	553.534	1159.266	813.307	204.546	−340.933	−16.7466
1700	509.198	604.229	1189.998	834.569	255.242	−338.909	−17.3993
1800	513.191	655.353	1219.219	855.134	306.366	−336.902	−17.9762
1900	516.683	706.851	1247.061	875.035	357.863	−334.941	−18.4892
2000	519.751	758.676	1273.643	894.305	409.688	−333.039	−18.9477
2100	522.459	810.789	1299.069	912.979	461.802	−331.219	−19.3611
2200	524.860	863.157	1323.430	931.086	514.170	−329.514	−19.7345
2300	526.997	915.752	1346.809	948.656	566.765	−327.912	−20.0739
2400	528.905	968.549	1369.279	965.717	619.562	−326.439	−20.3839
2500	530.616	1021.527	1390.905	982.295	672.539	−325.130	−20.6671
2600	532.156	1074.667	1411.747	998.414	725.679	−323.952	−20.9278
2700	533.545	1127.953	1431.857	1014.097	778.966	−322.951	−21.1687
2800	534.802	1181.371	1451.284	1029.366	832.384	−322.121	−21.3918
2900	535.944	1234.910	1470.071	1044.240	885.922	−321.469	−21.5984
3000	536.983	1288.557	1488.258	1058.740	939.569	−321.030	−21.7908
3100	537.931	1342.303	1505.882	1072.881	993.316	−320.750	−21.9716
3200	538.799	1396.140	1522.974	1086.680	1047.153	−320.686	−22.1405
3300	539.594	1450.060	1539.566	1100.154	1101.073	−320.820	−22.2989
3400	540.326	1504.057	1555.686	1113.316	1155.069	−321.153	−22.4482
3500	540.999	1558.124	1571.358	1126.180	1209.136	−321.704	−22.5897
3600	541.621	1612.255	1586.608	1138.759	1263.268	−322.437	−22.7229
3700	542.196	1666.446	1601.455	1151.065	1317.459	−323.386	−22.8498
3800	542.729	1720.693	1615.922	1163.108	1371.705	−324.529	−22.9697
3900	543.224	1774.991	1630.026	1174.900	1426.003	−325.861	−23.0846
4000	543.684	1829.336	1643.785	1186.451	1480.349	−327.409	−23.1936
4100	544.112	1883.726	1657.216	1197.770	1534.739	−329.114	−23.2987
4200	544.512	1938.158	1670.332	1208.866	1589.170	−331.013	−23.3989
4300	544.885	1992.628	1683.149	1219.747	1643.640	−333.103	−23.4944
4400	545.234	2047.134	1695.680	1230.422	1698.147	−335.397	−23.5862
4500	545.561	2101.674	1707.937	1240.898	1752.687	−337.824	−23.6751
4600	545.868	2156.246	1719.931	1251.182	1807.258	−340.403	−23.7605
4700	546.156	2210.847	1731.673	1261.280	1861.859	−343.123	−23.8431
4800	546.427	2265.476	1743.175	1271.201	1916.489	−345.982	−23.9233
4900	546.682	2320.132	1754.444	1280.948	1971.144	−348.976	−24.0008
5000	546.923	2374.812	1765.491	1290.529	2025.825	−352.218	−24.0749
5100	547.150	2429.516	1776.324	1299.948	2080.528	−355.445	−24.1483
5200	547.364	2484.242	1786.951	1309.212	2135.254	−358.875	−24.2186
5300	547.567	2538.988	1797.379	1318.325	2190.001	−362.424	−24.2869
5400	547.759	2593.755	1807.616	1327.291	2244.767	−366.094	−24.3535
5500	547.941	2648.540	1817.669	1336.116	2299.552	−369.876	−24.4182
5600	548.113	2703.342	1827.543	1344.803	2354.355	−373.768	−24.4812
5700	548.277	2758.162	1837.246	1353.358	2409.175	−377.767	−24.5427
5800	548.432	2812.998	1846.783	1361.783	2464.010	−381.869	−24.6027
5900	548.580	2867.848	1856.159	1370.083	2518.861	−386.070	−24.6613
6000	548.721	2922.713	1865.381	1378.262	2573.726	−390.364	−24.7186

TABLE 51. Molecular properties of $C_{12}H_5Cl_4O_2$· (2,4-dichlorophenoxy-1′,3′-dichlorophenyl-6-6′-ether radical). Values listed with bold characters were chosen for thermodynamic calculations—$\sigma = \mathbf{1}$ and statistical weight = **2**

	Enthalpy of formation $\Delta_f H°(298.15\ \text{K})$ / kcal mol^{-1}	Zero point energy ZPE / kcal mol^{-1}
Our estimate	**−20.44±6**	
NIST 94	−26.6	
PM3	−13.474	86.920
PM3-UHF	−24.979	86.216
AM1	−6.535	91.026

Moments of inertia of the molecule / g cm^2×10^{-39}

MOPAC method	I_a	I_b	I_c
PM3	**187.954 23**	**618.621 54**	**651.943 94**
PM3 UHF	171.691 56	597.983 69	681.586 36
AM1	165.321 24	603.132 14	666.366 14

Reduced moment of inertia[34] I_r(dcp) = **79.988** g cm^2×10^{-39}; $\sigma_{rot} = \mathbf{2}$; $V(2) = \mathbf{1116}$ cm^{-1}.
I_r(dcb) = **48.607** g cm^2×10^{-39}; $\sigma_{rot} = \mathbf{2}$; $V(2) = \mathbf{1116}$ cm^{-1}.

Molecular vibrations / cm^{-1}

PM3	12.43	17.37	**33.79**	**52.4**	**111**	**130**
	155	**161**	**174**	**195**	**214**	**257**
	284	**320**	**343**	**368**	**391**	**393**
	410	**444**	**482**	**502**	**534**	**540**
	571	**617**	**664**	**722**	**745**	**768**
	787	**857**	**879**	**905**	**913**	**928**
	935	**974**	**994**	**1065**	**1095**	**1128**
	1159	**1170**	**1186**	**1273**	**1300**	**1312**
	1382	**1409**	**1432**	**1523**	**1576**	**1644**
	1674	**1760**	**1773**	**1879**	**3036**	**3048**
	3054	**3060**	**3069**			
PM3 UHF	13.50	14.61	35	50.9	110	126
	153	158	164	195	213	254
	283	317	329	365	389	394
	409	442	469	482	508	531
	565	615	660	716	743	744
	783	849	864	871	885	905
	925	967	982	1062	1090	1126
	1151	1165	1184	1285	1340	1355
	1391	1423	1455	1511	1563	1572
	1604	1730	1743	1803	3039	3050
	3055	3058	3069			
AM1	11.58	19.86	43.14	52.29	110	132
	164	170	178	206	226	281
	303	333	353	403	423	441
	451	476	513	531	556	566
	596	651	709	760	776	848
	874	905	921	942	946	959
	977	990	1086	1164	1186	1206
	1251	1276	1285	1339	1361	1387
	1471	1472	1508	1545	1626	1668
	1702	1741	1757	1976	3163	3172
	3172	3181	3195			

TABLE 52. Thermodynamic properties of $C_{12}H_5Cl_4O_2$· (2,4-dichlorophenoxy-1′,3′-dichlorophenyl-6-6′-ether radical) (M_r=322.981)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	C_p° (J·K^{-1}·mol^{-1})	$H°-H°(T_r)$ (J·mol^{-1})	$S°$ (J·K^{-1}·mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}·mol^{-1})	$H(T)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	log K_f
0	—	−44.993	—	—	−130.514	−69.659	—
100	118.269	−37.130	391.026	762.323	−122.651	−78.756	19.0213
200	189.423	−21.658	495.433	603.725	−107.179	−82.930	−2.0249
298.15	250.467	0.000	582.730	582.730	−85.521	−85.521	−9.2586
300	251.530	0.464	584.282	582.735	−85.057	−85.560	−9.3509
400	303.456	28.305	664.018	593.254	−57.216	−87.174	−13.1098
500	344.685	60.796	736.348	614.755	−24.725	−88.111	−15.3993
600	376.895	96.941	802.159	640.590	11.420	−88.642	−16.9378
700	402.211	135.946	862.235	668.026	50.425	−88.850	−18.0417
800	422.386	177.213	917.309	695.793	91.692	−88.758	−18.8705
900	438.701	220.295	968.034	723.262	134.774	−88.373	−19.5132
1000	452.061	264.855	1014.970	750.115	179.334	−87.748	−20.0244
1100	463.119	310.631	1058.591	776.199	225.110	−86.911	−20.4393
1200	472.354	357.418	1099.295	801.447	271.897	−85.905	−20.7812
1300	480.129	405.053	1137.419	825.840	319.532	−84.780	−21.0676
1400	486.721	453.404	1173.248	849.388	367.883	−83.600	−21.3086
1500	492.346	502.365	1207.025	872.115	416.844	−82.360	−21.5158
1600	497.177	551.847	1238.959	894.054	466.326	−81.126	−21.6939
1700	501.348	601.778	1269.228	915.241	516.257	−79.923	−21.8485
1800	504.971	652.099	1297.989	935.712	566.578	−78.771	−21.9840
1900	508.132	702.757	1325.378	955.506	617.236	−77.692	−22.1034
2000	510.904	753.712	1351.514	974.658	668.191	−76.698	−22.2090
2100	513.347	804.927	1376.502	993.203	719.406	−75.808	−22.3042
2200	515.508	856.372	1400.433	1011.173	770.851	−75.054	−22.3893
2300	517.428	908.021	1423.392	1028.600	822.500	−74.423	−22.4665
2400	519.141	959.851	1445.450	1045.512	874.330	−73.939	−22.5372
2500	520.674	1011.843	1466.674	1061.937	926.322	−73.638	−22.6009
2600	522.052	1063.980	1487.123	1077.900	978.459	−73.486	−22.6599
2700	523.294	1116.249	1506.849	1093.423	1030.728	−73.528	−22.7149
2800	524.417	1168.635	1525.900	1108.531	1083.114	−73.761	−22.7660
2900	525.435	1221.128	1544.321	1123.242	1135.608	−74.191	−22.8131
3000	526.361	1273.719	1562.150	1137.577	1188.198	−74.851	−22.8574
3100	527.205	1326.398	1579.423	1151.553	1240.877	−75.689	−22.9003
3200	527.977	1379.158	1596.174	1165.187	1293.637	−76.762	−22.9404
3300	528.684	1431.991	1612.431	1178.495	1346.470	−78.051	−22.9785
3400	529.334	1484.893	1628.224	1191.491	1399.372	−79.556	−23.0150
3500	529.932	1537.856	1643.577	1204.189	1452.335	−81.296	−23.0507
3600	530.484	1590.877	1658.513	1216.603	1505.356	−83.235	−23.0845
3700	530.994	1643.952	1673.055	1228.744	1558.431	−85.402	−23.1178
3800	531.466	1697.075	1687.222	1240.623	1611.554	−87.777	−23.1496
3900	531.904	1750.244	1701.033	1252.252	1664.723	−90.353	−23.1813
4000	532.311	1803.455	1714.505	1263.641	1717.934	−93.153	−23.2116
4100	532.690	1856.705	1727.653	1274.799	1771.184	−96.118	−23.2422
4200	533.044	1909.992	1740.494	1285.734	1824.471	−99.283	−23.2720
4300	533.374	1963.313	1753.041	1296.457	1877.792	−102.642	−23.3007
4400	533.682	2016.666	1765.307	1306.973	1931.145	−106.206	−23.3289
4500	533.971	2070.049	1777.303	1317.292	1984.528	−109.901	−23.3576
4600	534.242	2123.459	1789.042	1327.421	2037.939	−113.746	−23.3856
4700	534.497	2176.897	1800.535	1337.365	2091.376	−117.726	−23.4136
4800	534.736	2230.358	1811.790	1347.132	2144.837	−121.839	−23.4418
4900	534.961	2283.843	1822.818	1356.728	2198.322	−126.077	−23.4696
5000	535.173	2337.350	1833.628	1366.158	2251.829	−130.554	−23.4963
5100	535.374	2390.878	1844.228	1375.428	2305.357	−135.002	−23.5245
5200	535.563	2444.424	1854.626	1384.544	2358.904	−139.641	−23.5514
5300	535.742	2497.990	1864.829	1393.510	2412.469	−144.383	−23.5783
5400	535.911	2551.572	1874.845	1402.331	2466.052	−149.229	−23.6052
5500	536.071	2605.172	1884.680	1411.012	2519.651	−154.171	−23.6319
5600	536.223	2658.786	1894.340	1419.557	2573.265	−159.205	−23.6584
5700	536.367	2712.416	1903.832	1427.970	2626.895	−164.326	−23.6850
5800	536.504	2766.060	1913.162	1436.255	2680.539	−169.532	−23.7113
5900	536.634	2819.717	1922.334	1444.416	2734.196	−174.816	−23.7375
6000	536.758	2873.386	1931.355	1452.457	2787.865	−180.173	−23.7637

TABLE 53. Molecular properties of $C_{12}H_5Cl_4O_3$· (1,3-dichloro-1-ol-2-yl-3,5,-cyclohexadiene-*p*-dioxin-6,8-dichlorobenzen radical). Values listed with bold characters were chosen for thermodynamic calculations—$\sigma = \mathbf{1}$ and statistical weight = **2**

	Enthalpy of formation $\Delta_f H°(298.15\ \mathrm{K})$ / kcal mol^{-1}	Zero point energy ZPE / kcal mol^{-1}
Our estimate	**−103.35±15**	
PM3	−53.662	91.137
PM3 UHF	−65.55	90.126
AM1	−35.988	94.685
AM1 UHF	−49.63	93.659

Moments of inertia of the molecule / g cm$^2\times10^{-39}$

MOPAC method	I_a	I_b	I_c
PM3	**190.562 5**	**565.817 15**	**723.242 22**
PM3 UHF	190.525 61	567.289 90	725.085 04
AM1	191.647 01	573.244 17	726.960 97
AM1 UHF	191.491 53	574.404 16	729.879 90

Reduced moment of inertia[36] $I_r(\mathrm{OH}) = \mathbf{0.1364}$ g cm$^2\times10^{-39}$; $\sigma_{\mathrm{rot}} = \mathbf{2}$; $V(2) = \mathbf{1116}$ cm^{-1}.

Molecular vibrations / cm^{-1}

PM3	**20.3**	**31.5**	**78.9**	**98.9**	**108.2**	**131**
	153.4	**168.6**	**177.4**	**194**	**217**	**247**
	275	**294**	**303**	**343**	**352**	**373**
	401	**414**	**460**	**485**	**511**	**536**
	541	**564**	**566**	**607**	**621**	**685**
	712	**731**	**765**	**855**	**878**	**885**
	913	**925**	**930**	**943**	**993**	**1101**
	1103	**1125**	**1173**	**1194**	**1247**	**1274**
	1317	**1327**	**1361**	**1379**	**1412**	**1440**
	1497	**1565**	**1608**	**1672**	**1775**	**1784**
	1788	**3056**	**3057**	**3061**	**3068**	**3887**
PM3 UHF	23	35.3	74.4	94	107	128
	153	167	175	193	214	245
	282	296	303	332	345	357
	401	406	455	479	485	509
	517	546	557	580	621	668
	696	709	762	824	840	858
	881	899	915	917	987	1096
	1099	1125	1172	1193	1259	1320
	1336	1354	1371	1397	1421	1445
	1503	1537	1572	1606	1615	1710
	1716	3057	3058	3061	3065	3887
AM1	13.8	30.5	82.4	99.7	119	137
	156	174	185	209	221	251
	290	317	332	358	380	404
	454	456	503	521	543	554
	557	578	594	627	674	709
	731	786	858	894	930	939
	944	956	965	1018	1098	1182
	1201	1213	1258	1271	1324	1357
	1376	1416	1438	1478	1491	1496
	1572	1602	1667	1715	1759	1777
	1784	3171	3183	3185	3197	3459
AM1 UHF	22.7	34.5	78.5	97.8	116	133
	156	171	182	208	220	249
	294	316	328	344	367	400
	443	451	496	512	516	529
	533	552	577	605	667	671
	718	778	843	849	878	906
	910	948	956	1008	1092	1173
	1196	1215	1262	1274	1347	1410
	1425	1441	1449	1481	1490	1507
	1565	1586	1619	1638	1669	1689
	1709	3174	3184	3191	3194	3459

TABLE 54. Thermodynamic properties of $C_{12}H_5Cl_4O_3$· (1,3-dichloro-1-ol-2-yl-3,5,-cyclohexadiene-*p*-dioxin-6,8-dichlorobenzene radical) (M_r=338.981)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	C_p° (J·K^{-1}·mol^{-1})	$H°-H°(T_r)$ (J·mol^{-1})	$S°$ (J·K^{-1}·mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}·mol^{-1})	$H(T)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	log K_f
0	—	−45.331	—	—	−477.747	−412.552	—
100	113.687	−38.579	353.314	739.104	−470.995	−424.211	192.9680
200	197.895	−22.848	458.994	573.235	−455.265	−429.581	81.5522
298.15	265.578	0.000	551.043	551.043	−432.416	−432.416	44.5016
300	266.735	0.492	552.689	551.048	−431.924	−432.455	44.0345
400	323.048	30.083	637.428	562.220	−402.333	−433.805	25.1798
500	367.740	64.713	714.517	585.091	−367.703	−434.133	13.8442
600	402.628	103.304	784.779	612.606	−329.113	−433.797	6.2879
700	429.933	144.986	848.979	641.856	−287.430	−432.955	0.8975
800	451.570	189.102	907.855	671.478	−243.314	−431.684	−3.1358
900	468.972	235.160	962.083	700.795	−197.257	−430.026	−6.2619
1000	483.168	282.790	1012.254	729.464	−149.627	−428.062	−8.7523
1100	494.891	331.711	1058.872	757.316	−100.705	−425.835	−10.7799
1200	504.674	381.704	1102.365	784.278	−50.713	−423.399	−12.4603
1300	512.911	432.594	1143.095	810.330	0.178	−420.811	−13.8743
1400	519.903	484.244	1181.368	835.479	51.828	−418.139	−15.0776
1500	525.878	536.541	1217.447	859.753	104.125	−415.385	−16.1151
1600	531.019	589.392	1251.554	883.184	156.976	−412.617	−17.0164
1700	535.467	642.722	1283.884	905.812	210.305	−409.863	−17.8060
1800	539.338	696.466	1314.602	927.677	264.050	−407.146	−18.5034
1900	542.722	750.573	1343.856	948.817	318.157	−404.490	−19.1232
2000	545.696	804.997	1371.771	969.272	372.581	−401.910	−19.6769
2100	548.322	859.701	1398.460	989.079	427.284	−399.427	−20.1756
2200	550.649	914.652	1424.023	1008.272	482.235	−397.073	−20.6256
2300	552.720	969.822	1448.547	1026.885	537.406	−394.838	−21.0345
2400	554.570	1025.188	1472.110	1044.948	592.772	−392.747	−21.4076
2500	556.229	1080.730	1494.783	1062.491	648.313	−390.838	−21.7482
2600	557.721	1136.428	1516.628	1079.541	704.012	−389.077	−22.0614
2700	559.068	1192.269	1537.703	1096.122	759.853	−387.509	−22.3506
2800	560.287	1248.238	1558.057	1112.258	815.821	−386.133	−22.6182
2900	561.394	1304.323	1577.738	1127.971	871.906	−384.955	−22.8657
3000	562.402	1360.513	1596.787	1143.283	928.097	−384.010	−23.0961
3100	563.321	1416.800	1615.244	1158.211	984.384	−383.244	−23.3122
3200	564.163	1473.175	1633.142	1172.775	1040.759	−382.716	−23.5138
3300	564.934	1529.630	1650.514	1186.990	1097.214	−382.406	−23.7028
3400	565.644	1586.160	1667.390	1200.872	1153.743	−382.316	−23.8807
3500	566.297	1642.757	1683.796	1214.437	1210.341	−382.463	−24.0489
3600	566.900	1699.418	1699.757	1227.697	1267.001	−382.813	−24.2072
3700	567.458	1756.136	1715.298	1240.666	1323.719	−383.394	−24.3577
3800	567.975	1812.908	1730.438	1253.357	1380.491	−384.187	−24.4999
3900	568.455	1869.730	1745.197	1265.780	1437.313	−385.183	−24.6358
4000	568.901	1926.598	1759.595	1277.946	1494.181	−386.408	−24.7645
4100	569.317	1983.509	1773.648	1289.865	1551.092	−387.801	−24.8883
4200	569.704	2040.460	1787.372	1301.548	1608.044	−389.398	−25.0063
4300	570.066	2097.449	1800.781	1313.003	1665.032	−391.191	−25.1187
4400	570.405	2154.473	1813.891	1324.238	1722.056	−393.194	−25.2264
4500	570.722	2211.529	1826.713	1335.262	1779.113	−395.332	−25.3306
4600	571.020	2268.616	1839.260	1346.083	1836.200	−397.624	−25.4305
4700	571.299	2325.732	1851.544	1356.707	1893.316	−400.054	−25.5268
4800	571.562	2382.876	1863.574	1367.142	1950.459	−402.621	−25.6202
4900	571.810	2440.044	1875.362	1377.394	2007.628	−405.317	−25.7102
5000	572.043	2497.237	1886.917	1387.469	2064.821	−408.254	−25.7963
5100	572.264	2554.453	1898.247	1397.374	2122.036	−411.167	−25.8812
5200	572.472	2611.689	1909.361	1407.113	2179.273	−414.274	−25.9624
5300	572.668	2668.947	1920.268	1416.693	2236.530	−417.487	−26.0412
5400	572.855	2726.223	1930.974	1426.118	2293.806	−420.809	−26.1178
5500	573.031	2783.517	1941.487	1435.393	2351.101	−424.229	−26.1921
5600	573.198	2840.829	1951.813	1444.523	2408.412	−427.744	−26.2643
5700	573.357	2898.157	1961.960	1453.512	2465.740	−431.350	−26.3346
5800	573.508	2955.500	1971.933	1462.364	2523.084	−435.043	−26.4031
5900	573.652	3012.858	1981.738	1471.084	2580.442	−438.818	−26.4696
6000	573.788	3070.230	1991.381	1479.676	2637.814	−442.667	−26.5347

TABLE 55. Molecular properties of $\cdot C_{12}H_5Cl_4O_3$ (1,3,-dichloro-2-ol-3-yl-1,4-cyclohexadiene-*p*-dioxin-6,8-dichlorobenzene radical). Values listed with bold characters were chosen for thermodynamic calculations—$\sigma = \mathbf{1}$ and statistical weight = **2**

	Enthalpy of formation $\Delta_f H°(298.15\ \mathrm{K})$ / kcal mol^{-1}	Zero point energy ZPE / kcal mol^{-1}
Our estimate	**−76.91±15**	
PM3	−55.04	91.101
PM3 UHF	−66.93	90.214
AM1 UHF	−55.51	94.247

Moments of inertia of the molecule / g cm^2×10^{-39}

MOPAC method	I_a	I_b	I_c
PM3	**187.929 1**	**582.179 79**	**756.073 31**
PM3 UHF	185.239 3	589.553 88	770.966 83
AM1 UHF	187.834 74	596.779 18	781.711 24

Reduced moment of inertia[36] $I_r(\mathrm{OH}) = \mathbf{0.1364}$ g cm^2×10^{-39}; $\sigma_{\mathrm{rot}} = \mathbf{2}$; $V(2) = \mathbf{1116}$ cm^{-1}.

Molecular vibrations / cm^{-1}

PM3	25.41	**43.59**	**58.3**	**92.1**	**119**	**149**
	156	**166**	**192**	**198**	**204**	**228**
	264	**274**	**309**	**344**	**349**	**365**
	372	**401**	**449**	**474**	**512**	**535**
	566	**576**	**620**	**623**	**666**	**716**
	727	**735**	**804**	**839**	**900**	**917**
	922	**941**	**953**	**1011**	**1014**	**1044**
	1090	**1111**	**1174**	**1204**	**1301**	**1308**
	1325	**1335**	**1348**	**1359**	**1370**	**1415**
	1514	**1565**	**1616**	**1653**	**1745**	**1785**
	1791	**2852**	**3051**	**3059**	**3062**	**3888**
PM3 UHF	25.58	34	46.79	102.6	105.2	144
	157	159	191	195	198	234
	256	298	304	331	347	355
	372	399	446	448	506	517
	546	565	592	623	639	696
	712	719	799	835	871	889
	898	914	948	1003	1010	1036
	1087	1104	1172	1204	1302	1318
	1330	1356	1360	1368	1392	1493
	1513	1534	1577	1591	1606	1713
	1718	2852	3052	3059	3063	3890
AM1 UHF	20.23	29.2	39.7	98.5	114.2	144.4
	157	172.8	194	211	215	249
	292	325	341	342	362	384
	406	450	466	491	527	537
	553	577	612	666	669	674
	754	815	887	888	907	911
	930	965	1048	1121	1140	1186
	1207	1250	1262	1293	1367	1399
	1426	1442	1448	1452	1515	1525
	1561	1589	1614	1641	1656	1697
	1713	2970	3176	3176	3191	3482

TABLE 56. Thermodynamic properties of ·$C_{12}H_5Cl_4O_3$ (1,3,-dichloro-2-ol-3-yl-1,4-cyclohexadiene-*p*-dioxin-6,8-dichlorobenzene radical) (M_r=338.977)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	C_p° (J·K^{-1}·mol^{-1})	$H°-H°(T_r)$ (J·mol^{-1})	$S°$ (J·K^{-1}·mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}·mol^{-1})	$H(T)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	log K_f
0	—	−45.226	—	—	−367.018	−301.823	—
100	114.481	−38.469	352.693	737.382	−360.260	−313.476	135.0949
200	197.185	−22.713	458.615	572.178	−344.504	−318.821	52.6055
298.15	263.787	0.000	550.127	550.127	−321.791	−321.791	25.0732
300	264.937	0.489	551.762	550.132	−321.302	−321.833	24.7257
400	321.278	29.896	635.973	561.232	−291.895	−323.367	10.6824
500	366.327	64.366	712.703	583.971	−257.425	−323.855	2.2291
600	401.601	102.835	782.743	611.351	−218.956	−323.641	−3.4082
700	429.239	144.432	846.810	640.478	−177.359	−322.885	−7.4292
800	451.139	188.492	905.612	669.996	−133.299	−321.669	−10.4361
900	468.739	234.517	959.801	699.226	−87.274	−320.043	−12.7642
1000	483.078	282.132	1009.954	727.823	−39.660	−318.095	−14.6163
1100	494.902	331.049	1056.569	755.615	9.258	−315.872	−16.1218
1200	504.754	381.046	1100.066	782.527	59.255	−313.431	−17.3670
1300	513.038	431.948	1140.804	808.537	110.156	−310.832	−18.4128
1400	520.059	483.612	1179.088	833.651	161.821	−308.147	−19.3004
1500	526.052	535.925	1215.178	857.895	214.134	−305.376	−20.0643
1600	531.202	588.794	1249.298	881.301	267.003	−302.590	−20.7262
1700	535.654	642.143	1281.638	903.907	320.351	−299.817	−21.3046
1800	539.524	695.906	1312.368	925.753	374.115	−297.082	−21.8141
1900	542.906	750.031	1341.631	946.877	428.240	−294.407	−22.2657
2000	545.875	804.473	1369.555	967.319	482.682	−291.809	−22.6681
2100	548.495	859.195	1396.253	987.113	537.403	−289.308	−23.0298
2200	550.815	914.162	1421.824	1006.296	592.371	−286.937	−23.3554
2300	552.880	969.349	1446.355	1024.899	647.558	−284.686	−23.6505
2400	554.723	1024.731	1469.925	1042.954	702.940	−282.580	−23.9194
2500	556.375	1080.287	1492.604	1060.489	758.496	−280.655	−24.1641
2600	557.861	1136.001	1514.455	1077.532	814.209	−278.880	−24.3888
2700	559.201	1191.855	1535.534	1094.107	870.063	−277.299	−24.5960
2800	560.414	1247.837	1555.894	1110.238	926.045	−275.910	−24.7874
2900	561.515	1303.934	1575.579	1125.946	982.142	−274.719	−24.9640
3000	562.517	1360.136	1594.632	1141.253	1038.345	−273.762	−25.1282
3100	563.431	1416.434	1613.092	1156.178	1094.643	−272.985	−25.2823
3200	564.268	1472.820	1630.994	1170.737	1151.028	−272.446	−25.4259
3300	565.035	1529.286	1648.369	1184.949	1207.494	−272.126	−25.5604
3400	565.739	1585.825	1665.248	1198.829	1264.033	−272.026	−25.6869
3500	566.389	1642.432	1681.657	1212.390	1320.640	−272.164	−25.8067
3600	566.988	1699.101	1697.621	1225.648	1377.309	−272.504	−25.9193
3700	567.542	1755.828	1713.163	1238.615	1434.036	−273.077	−26.0266
3800	568.055	1812.608	1728.305	1251.303	1490.816	−273.862	−26.1278
3900	568.531	1869.437	1743.067	1263.724	1547.646	−274.851	−26.2247
4000	568.974	1926.313	1757.467	1275.889	1604.521	−276.068	−26.3166
4100	569.387	1983.231	1771.521	1287.806	1661.440	−277.453	−26.4052
4200	569.772	2040.189	1785.247	1299.488	1718.398	−279.043	−26.4897
4300	570.131	2097.185	1798.658	1310.941	1775.393	−280.831	−26.5702
4400	570.467	2154.215	1811.769	1322.175	1832.423	−282.827	−26.6474
4500	570.782	2211.277	1824.593	1333.198	1889.486	−284.959	−26.7225
4600	571.077	2268.371	1837.141	1344.017	1946.579	−287.245	−26.7945
4700	571.355	2325.492	1849.426	1354.640	2003.701	−289.670	−26.8642
4800	571.616	2382.641	1861.458	1365.074	2060.850	−292.230	−26.9320
4900	571.861	2439.815	1873.246	1375.325	2118.024	−294.921	−26.9975
5000	572.093	2497.013	1884.802	1385.399	2175.221	−297.853	−27.0601
5100	572.312	2554.233	1896.133	1395.303	2232.442	−300.762	−27.1223
5200	572.518	2611.475	1907.248	1405.042	2289.683	−303.863	−27.1818
5300	572.713	2668.736	1918.156	1414.620	2346.945	−307.073	−27.2396
5400	572.898	2726.017	1928.863	1424.045	2404.226	−310.390	−27.2961
5500	573.073	2783.316	1939.376	1433.319	2461.524	−313.806	−27.3510
5600	573.239	2840.631	1949.704	1442.448	2518.840	−317.317	−27.4045
5700	573.396	2897.963	1959.851	1451.437	2576.172	−320.918	−27.4567
5800	573.546	2955.310	1969.825	1460.289	2633.519	−324.608	−27.5077
5900	573.688	3012.672	1979.631	1469.008	2690.881	−328.379	−27.5575
6000	573.824	3070.048	1989.274	1477.599	2748.256	−332.224	−27.6062

TABLE 57. Molecular properties of $C_{12}H_5Cl_5O_2$ (2,4-dichlorophenol-1′,3′,5′-trichlorophenyl-6-6′-ether–$Cl_2C_6H_2(OH)-O-C_6H_2Cl_3$). Values listed with bold characters were chosen for thermodynamic calculations—$\sigma = \mathbf{1}$ and statistical weight = **1**

	Enthalpy of formation $\Delta_f H°(298.15\ \mathrm{K})$ / kcal mol^{-1}	Zero point energy ZPE / kcal mol^{-1}
Our estimate	**−59.79±5**	
NIST 94	−67.4	
PM3	−50.80	89.755
PM3 UHF	−49.96	88.907
AM1	−44.19	92.140
AM1 UHF	−43.24	93.027

Moments of inertia of the molecule / g cm$^2\times10^{-39}$

MOPAC method	I_a	I_b	I_c
PM3	**236.939 34**	**577.550 84**	**706.860 84**
PM3 UHF	231.814 92	588.289 92	700.566 99
AM1	223.335 42	656.511 75	678.751 77
AM1 UHF	223.089 67	649.018 79	680.025 74

Reduced moment of inertia[34] I_r(OH) = **0.1364** g cm$^2\times10^{-39}$; $\sigma_{rot} = \mathbf{2}$; $V(2) = \mathbf{1116}$ cm^{-1}.
I_r(tcb) = **84.797** g cm$^2\times10^{-39}$; $\sigma_{rot} = \mathbf{2}$; $V(2) = \mathbf{1116}$ cm^{-1}.
I_r(dcp) = **73.905** g cm$^2\times10^{-39}$; $\sigma_{rot} = \mathbf{2}$; $V(2) = \mathbf{1116}$ cm^{-1}.

Molecular vibrations / cm^{-1}

PM3	14.07	18.62	32.15	**76.9**	**83.2**	**139**
	142	**151**	**180**	**186**	**191**	**196**
	217	**272**	**297**	**316**	**336**	**357**
	371	**375**	**406**	**424**	**435**	**521**
	530	**534**	**552**	**565**	**573**	**618**
	729	**737**	**747**	**789**	**816**	**895**
	908	**921**	**926**	**939**	**949**	**996**
	1081	**1107**	**1159**	**1174**	**1200**	**1292**
	1330	**1347**	**1384**	**1429**	**1451**	**1515**
	1565	**1581**	**1623**	**1752**	**1767**	**1773**
	1781	**3045**	**3053**	**3058**	**3062**	**3855**
PM3 UHF	20.66	27.6	45.8	82.9	95.8	136
	142	151	179	188	192	197
	221	269	285	317	342	352
	370	371	398	422	426	485
	516	534	546	549	580	633
	710	723	754	782	802	879
	886	911	915	929	933	977
	1077	1096	1157	1161	1171	1285
	1326	1339	1364	1387	1418	1496
	1540	1556	1594	1708	1714	1720
	1734	3052	3055	3058	3059	3845
AM1	9.18	17.8	31.9	76.2	86.5	142
	147	159	188	189	201	207
	234	262	289	317	325	368
	415	438	454	465	469	545
	557	567	577	583	607	642
	714	777	854	900	915	931
	940	944	946	975	982	1097
	1191	1214	1253	1261	1314	1372
	1376	1413	1472	1486	1527	1541
	1609	1628	1691	1730	1745	1770
	1772	3172	3175	3178	3181	3409
AM1 UHF	7.97	23.77	32.18	76.06	81.5	139
	145	159	182	184	199	209
	234	236	289	311	349	357
	412	436	451	461	465	527
	543	553	558	573	598	634
	682	762	848	895	909	914
	919	929	932	965	974	1092
	1087	1210	1258	1264	1298	1383
	1408	1422	1451	1471	1515	1519
	1592	1605	1669	1673	1690	1709
	1730	3167	3170	3172	3178	3425

TABLE 58. Thermodynamic properties of $C_{12}H_5Cl_5O_2$ (2,4-dichlorophenol-1′,3′,5′-trichlorophenyl-6-6′-ether) (M_r=358.434)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	$C_p°$ (J·K^{-1}·mol^{-1})	$H°-H°(T_r)$ (J·mol^{-1})	$S°$ (J·K^{-1}·mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}·mol^{-1})	$H(T)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	log K_f
0	—	−47.711	—	—	−297.872	−232.427	—
100	122.687	−40.093	379.465	780.393	−290.254	−243.224	99.3887
200	205.729	−23.495	491.202	608.677	−273.656	−247.791	35.3268
298.15	270.758	0.000	585.917	585.917	−250.161	−250.161	13.9253
300	271.856	0.502	587.596	585.923	−249.659	−250.194	13.6551
400	324.646	30.432	673.335	597.255	−219.729	−251.455	2.7370
500	365.848	65.044	750.398	620.310	−185.117	−252.056	−3.8388
600	397.810	103.294	820.047	647.891	−146.868	−252.298	−8.2293
700	422.826	144.375	883.325	677.075	−105.786	−252.266	−11.3671
800	442.709	187.688	941.132	706.522	−62.473	−251.977	−13.7192
900	458.770	232.790	994.236	735.580	−17.371	−251.432	−15.5455
1000	471.927	279.346	1043.275	763.929	29.184	−250.680	−17.0027
1100	482.837	327.101	1088.782	791.418	76.939	−249.740	−18.1909
1200	491.973	375.854	1131.197	817.985	125.693	−248.648	−19.1771
1300	499.690	425.448	1170.889	843.622	175.287	−247.451	−20.0082
1400	506.256	475.754	1208.167	868.343	225.593	−246.208	−20.7159
1500	511.881	526.668	1243.292	892.180	276.507	−244.910	−21.3275
1600	516.728	578.104	1276.486	915.171	327.943	−243.622	−21.8594
1700	520.929	629.992	1307.942	937.358	379.831	−242.368	−22.3260
1800	524.589	682.272	1337.823	958.783	432.111	−241.167	−22.7387
1900	527.793	734.895	1366.274	979.488	484.733	−240.038	−23.1061
2000	530.611	787.818	1393.420	999.511	537.656	−238.996	−23.4348
2100	533.101	841.006	1419.370	1018.891	590.844	−238.060	−23.7318
2200	535.309	894.428	1444.221	1037.663	644.267	−237.262	−24.0003
2300	537.276	948.060	1468.061	1055.861	697.898	−236.590	−24.2450
2400	539.034	1001.877	1490.965	1073.517	751.715	−236.072	−24.4691
2500	540.610	1055.860	1513.002	1090.658	805.699	−235.743	−24.6739
2600	542.029	1109.993	1534.233	1107.313	859.832	−235.571	−24.8632
2700	543.311	1164.262	1554.714	1123.506	914.100	−235.602	−25.0387
2800	544.471	1218.652	1574.494	1139.262	968.490	−235.835	−25.2019
2900	545.524	1273.152	1593.619	1154.601	1022.991	−236.277	−25.3533
3000	546.484	1327.753	1612.130	1169.545	1077.592	−236.964	−25.4949
3100	547.360	1382.446	1630.063	1184.113	1132.285	−237.844	−25.6288
3200	548.161	1437.223	1647.454	1198.322	1187.061	−238.973	−25.7544
3300	548.897	1492.076	1664.334	1212.189	1241.915	−240.333	−25.8727
3400	549.572	1547.000	1680.730	1225.730	1296.839	−241.925	−25.9847
3500	550.195	1601.989	1696.670	1238.959	1351.828	−243.768	−26.0917
3600	550.770	1657.038	1712.177	1251.889	1406.876	−245.824	−26.1929
3700	551.302	1712.142	1727.275	1264.534	1461.980	−248.121	−26.2900
3800	551.795	1767.297	1741.984	1276.906	1517.135	−250.640	−26.3823
3900	552.252	1822.499	1756.323	1289.016	1572.338	−253.370	−26.4713
4000	552.678	1877.746	1770.311	1300.874	1627.585	−256.334	−26.556
4100	553.074	1933.034	1783.963	1312.491	1682.873	−259.470	−26.6389
4200	553.444	1988.360	1797.295	1323.876	1738.199	−262.813	−26.7183
4300	553.789	2043.722	1810.322	1335.037	1793.561	−266.353	−26.7943
4400	554.112	2099.117	1823.057	1345.985	1848.956	−270.101	−26.8678
4500	554.415	2154.544	1835.513	1356.725	1904.382	−273.981	−26.9397
4600	554.699	2210.000	1847.701	1367.267	1959.838	−278.009	−27.0092
4700	554.966	2265.483	1859.634	1377.616	2015.322	−282.168	−27.0768
4800	555.217	2320.992	1871.320	1387.780	2070.831	−286.455	−27.1431
4900	555.453	2376.526	1882.771	1397.766	2126.364	−290.859	−27.2075
5000	555.676	2432.082	1893.995	1407.578	2181.921	−295.494	−27.2694
5100	555.886	2487.661	1905.001	1417.224	2237.499	−300.089	−27.3313
5200	556.085	2543.259	1915.797	1426.709	2293.098	−304.863	−27.3908
5300	556.273	2598.877	1926.391	1436.037	2348.716	−309.728	−27.4490
5400	556.450	2654.513	1936.791	1445.214	2404.352	−314.683	−27.5061
5500	556.619	2710.167	1947.003	1454.245	2460.006	−319.718	−27.5619
5600	556.779	2765.837	1957.033	1463.134	2515.676	−324.828	−27.6165
5700	556.930	2821.522	1966.890	1471.886	2571.361	−330.009	−27.6701
5800	557.074	2877.223	1976.577	1480.504	2627.061	−335.256	−27.7227
5900	557.211	2932.937	1986.101	1488.993	2682.776	−340.565	−27.7741
6000	557.342	2988.665	1995.467	1497.356	2738.503	−345.926	−27.8248

TABLE 59. Molecular properties of $C_{12}H_6Cl_4O_2$ (2,4-dichloro-phenol-1′3′-dichloro-phenyl-6-2′-ether–$Cl_2C_6H_2(OH)–O–C_6H_3Cl_2$). Values listed with bold characters were chosen for thermodynamic calculations—$\sigma = \mathbf{1}$ and statistical weight = **1**

	Enthalpy of formation $\Delta_f H°(298.15\ K)$ / kcal mol^{-1}	Zero point energy ZPE / kcal mol^{-1}
Our estimate	**−49.61**	
NIST 94	−60.3	
PM3	−46.12	95.418

Moments of inertia of the molecule / g cm$^2 \times 10^{-39}$

MOPAC method	I_a	I_b	I_c
PM3	**200.857 843 2**	**625.366 06**	**651.147 57**

Reduced moment of inertia[34] $I_r(OH) = \mathbf{0.1369}$ g cm$^2 \times 10^{-39}$; $\sigma_{rot} = \mathbf{2}$; $V(2) = \mathbf{1116}$ cm^{-1}.
$I_r(dcph) = \mathbf{79.918}$ g cm$^2 \times 10^{-39}$; $\sigma_{rot} = \mathbf{2}$; $V(2) = \mathbf{1116}$ cm^{-1}.
$I_r(dcb) = \mathbf{48.608}$ g cm$^2 \times 10^{-39}$; $\sigma_{rot} = \mathbf{2}$; $V(2) = \mathbf{1116}$ cm^{-1}.

Molecular vibrations / cm^{-1}

PM3	13.1	13.5	44.1	**85.4**	**97.2**	**142**
	153	**160**	**194**	**197**	**240**	**251**
	272	**306**	**338**	**343**	**373**	**386**
	401	**402**	**418**	**455**	**528**	**554**
	557	**587**	**644**	**673**	**706**	**735**
	750	**790**	**849**	**884**	**894**	**934**
	935	**955**	**977**	**1000**	**1067**	**1101**
	1138	**1161**	**1170**	**1197**	**1273**	**1323**
	1335	**1387**	**1416**	**1426**	**1535**	**1561**
	1576	**1617**	**1764**	**1768**	**1772**	**1781**
	3049	**3054**	**3057**	**3058**	**3066**	**3850**

TABLE 60. Thermodynamic properties of $C_{12}H_6Cl_4O_2$ (2,4-dichloro-phenol-1′,3′-dichloro-phenyl-6-2′-ether) (M_r=323.986)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	C_p° ($J\cdot K^{-1}\cdot mol^{-1}$)	$H°-H°(T_r)$ ($J\cdot mol^{-1}$)	$S°$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$-[G°-H°(T_r)]/T$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$H(T)$ ($kJ\cdot mol^{-1}$)	$\Delta_f H°$ ($kJ\cdot mol^{-1}$)	log K_f
0	—	−44.729	—	—	−252.297	−187.209	—
100	113.174	−37.575	368.438	744.187	−245.143	−198.514	77.7643
200	192.509	−22.143	472.241	582.957	−229.711	−204.075	25.2839
298.15	256.821	0.000	561.466	561.466	−207.568	−207.568	7.5994
300	257.924	0.476	563.059	561.471	−207.092	−207.622	7.3752
400	311.476	29.046	644.878	572.264	−178.523	−209.961	−1.7116
500	353.730	62.393	719.115	594.329	−145.175	−211.503	−7.2153
600	386.709	99.482	786.646	620.842	−108.086	−212.553	−10.9065
700	412.676	139.501	848.284	648.996	−68.067	−213.216	−13.5542
800	433.455	181.845	904.795	677.489	−25.723	−213.524	−15.5449
900	450.354	226.064	956.858	705.676	18.495	−213.489	−17.0940
1000	464.291	271.817	1005.051	733.234	64.249	−213.172	−18.3322
1100	475.915	318.845	1049.864	760.005	111.277	−212.603	−19.3432
1200	485.699	366.939	1091.706	785.923	159.371	−211.829	−20.1830
1300	493.998	415.935	1130.919	810.969	208.367	−210.904	−20.8913
1400	501.086	465.698	1167.794	835.153	258.130	−209.893	−21.4945
1500	507.175	516.119	1202.579	858.499	308.551	−208.798	−22.0160
1600	512.436	567.106	1235.483	881.042	359.538	−207.684	−22.4695
1700	517.006	618.583	1266.690	902.817	411.015	−206.582	−22.8672
1800	520.993	670.488	1296.356	923.863	462.920	−205.513	−23.2190
1900	524.490	722.766	1324.621	944.218	515.197	−204.501	−23.5320
2000	527.569	775.372	1351.603	963.917	567.804	−203.561	−23.8120
2100	530.292	828.268	1377.411	982.998	620.699	−202.712	−24.0650
2200	532.710	881.420	1402.137	1001.491	673.852	−201.990	−24.2935
2300	534.865	934.801	1425.865	1019.430	727.233	−201.381	−24.5018
2400	536.793	988.386	1448.670	1036.843	780.817	−200.914	−24.6926
2500	538.523	1042.153	1470.619	1053.758	834.585	−200.623	−24.8669
2600	540.081	1096.084	1491.771	1070.200	888.516	−200.476	−25.0279
2700	541.488	1150.164	1512.181	1086.194	942.596	−200.518	−25.1774
2800	542.763	1204.378	1531.897	1101.762	996.809	−200.748	−25.3163
2900	543.921	1258.713	1550.964	1116.925	1051.144	−201.172	−25.4451
3000	544.976	1313.158	1569.421	1131.702	1105.590	−201.826	−25.5656
3100	545.939	1367.705	1587.307	1146.112	1160.137	−202.656	−25.6798
3200	546.821	1422.343	1604.654	1160.172	1214.775	−203.720	−25.7868
3300	547.630	1477.067	1621.493	1173.897	1269.498	−205.000	−25.8876
3400	548.374	1531.867	1637.853	1187.303	1324.299	−206.497	−25.9832
3500	549.060	1586.740	1653.759	1200.405	1379.171	−208.230	−26.0747
3600	549.693	1641.678	1669.235	1213.214	1434.109	−210.163	−26.1611
3700	550.279	1696.677	1684.304	1225.743	1489.108	−212.327	−26.2442
3800	550.822	1751.732	1698.987	1238.005	1544.164	−214.701	−26.3231
3900	551.326	1806.840	1713.301	1250.009	1599.271	−217.278	−26.3995
4000	551.795	1861.996	1727.265	1261.766	1654.428	−220.083	−26.4723
4100	552.231	1917.197	1740.896	1273.287	1709.629	−223.055	−26.5434
4200	552.639	1972.441	1754.209	1284.580	1764.873	−226.231	−26.6116
4300	553.019	2027.724	1767.217	1295.653	1820.156	−229.605	−26.6770
4400	553.376	2083.044	1779.935	1306.516	1875.476	−233.188	−26.7404
4500	553.709	2138.399	1792.374	1317.175	1930.830	−236.906	−26.8025
4600	554.023	2193.786	1804.548	1327.638	1986.217	−240.778	−26.8627
4700	554.317	2249.203	1816.466	1337.912	2041.634	−244.790	−26.9213
4800	554.594	2304.648	1828.139	1348.004	2097.080	−248.939	−26.9789
4900	554.854	2360.121	1839.577	1357.920	2152.553	−253.218	−27.0350
5000	555.100	2415.619	1850.789	1367.665	2208.050	−257.740	−27.0888
5100	555.332	2471.140	1861.784	1377.247	2263.572	−262.238	−27.1430
5200	555.551	2526.685	1872.570	1386.669	2319.116	−266.929	−27.1950
5300	555.758	2582.250	1883.154	1395.937	2374.682	−271.730	−27.2460
5400	555.954	2637.836	1893.544	1405.056	2430.267	−276.637	−27.2962
5500	556.140	2693.440	1903.747	1414.030	2485.872	−281.644	−27.3453
5600	556.316	2749.063	1913.769	1422.865	2541.495	−286.747	−27.3934
5700	556.483	2804.703	1923.617	1431.564	2597.135	−291.940	−27.4408
5800	556.642	2860.360	1933.297	1440.131	2652.791	−297.221	−27.4874
5900	556.793	2916.032	1942.814	1448.571	2708.463	−302.584	−27.5330
6000	556.937	2971.718	1952.173	1456.887	2764.150	−308.020	−27.5781

TABLE 61. Molecular properties of $C_{12}H_8O$ (dibenzofuran). Values listed with bold characters were chosen for thermodynamic calculations—$\sigma = \mathbf{2}$ and statistical weight = **1**

	Enthalpy of formation $\Delta_f H°(298.15\ \mathrm{K})$ / kcal mol^{-1}	Zero point energy ZPE / kcal mol^{-1}
Chirico[52]	**13.19±0.1**	
NIST 2000[26]	11.30±1.1	
PM3	26.08	103.011

Moments of inertia of the molecule / g cm^2×10^{-39}

MOPAC method	I_a	I_b	I_c
Dorofeeva[48]	**31.1705**	**139.729 09**	**176.8996**
PM3	37.5060	138.945 21	176.4376

Molecular vibrations / cm^{-1}

IR[26]						
					562	589
	616	657	675		720	751
				841	859	931
			1003	1017		
	1115	1151	1196		1237	
	1286	1313		1439	1525	1534
	1597	1668	1695	1772	1808	1853
	1889	1929	2819	2918	3062	
Dorofeeva[48]	**118**	**138**	**244**	**289**	**322**	**406**
	430	**458**	**500**	**518**	**579**	**597**
	617	**623**	**674**	**705**	**738**	**752**
	796	**823**	**832**	**842**	**888**	**949**
	970	**986**	**1007**	**1010**	**1011**	**1048**
	1107	**1123**	**1171(2)**[a]	**1209**	**1247**	**1261**
	1290	**1305**	**1385**	**1389**	**1416**	**1444**
	1499	**1510**	**1564**	**1584**	**1601**	**1622**
	3050(4)[a]	**3053(4)**[a]				
PM3	112.4	153.3	232	269	280	399
	433	456	509	522	539	554
	634	674	700	770	798	806
	823	883	900	907	913	972
	976	1015	1018	1058	1087	1105
	1121	1140	1160	1161	1198	1211
	1303	1336(2)	1346	1426	1532	1558
	1596	1645	1768	1793	1819	1842
	3016(2)	3027(2)	3042	3043	3047(2)	

[a]Numbers in parenthesis show multiplicity.

TABLE 62. Thermodynamic properties of $C_{12}H_8O$ (dibenzofuran) (M_r=168.195)

Enthalpy Reference Temperature=T_r=298.15 K				Standard State Pressure=$p°$=0.1 MPa			
T (K)	C_p° ($J\cdot K^{-1}\cdot mol^{-1}$)	$H°-H°(T_r)$ ($J\cdot mol^{-1}$)	$S°$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$-[G°-H°(T_r)]/T$ ($J\cdot K^{-1}\cdot mol^{-1}$)	$H(T)$ ($kJ\cdot mol^{-1}$)	$\Delta_f H°$ ($kJ\cdot mol^{-1}$)	log K_f
0	—	−25.229	—	—	29.958	80.812	—
100	56.401	−21.095	269.479	480.424	34.092	70.763	−49.0469
200	105.227	−13.171	322.470	388.324	42.016	62.532	−31.4174
298.15	163.566	0.000	375.274	375.274	55.187	55.187	−26.3220
300	164.667	0.304	376.289	375.277	55.491	55.061	−26.2625
400	220.782	19.642	431.533	382.429	74.829	49.012	−23.9902
500	267.511	44.140	486.007	397.726	99.327	44.370	−22.7693
600	304.771	72.826	538.204	416.827	128.013	40.831	−22.0266
700	334.435	104.842	587.497	437.723	160.029	38.198	−21.5352
800	358.360	139.523	633.772	459.368	194.710	36.343	−21.1881
900	377.943	176.369	677.148	481.182	231.556	35.175	−20.9288
1000	394.172	215.000	717.834	502.835	270.187	34.570	−20.7264
1100	407.755	255.116	756.059	524.135	310.303	34.447	−20.5628
1200	419.212	296.480	792.043	544.976	351.667	34.712	−20.4260
1300	428.942	338.901	825.993	565.300	394.088	35.280	−20.3094
1400	437.253	382.221	858.093	585.078	437.408	36.056	−20.2064
1500	444.393	426.312	888.510	604.301	481.499	37.018	−20.1164
1600	450.557	471.067	917.392	622.975	526.254	38.086	−20.0350
1700	455.907	516.397	944.871	641.108	571.584	39.212	−19.9606
1800	460.571	562.226	971.065	658.717	617.413	40.373	−19.8927
1900	464.656	608.492	996.078	675.820	663.679	41.531	−19.8303
2000	468.250	655.141	1020.006	692.435	710.328	42.669	−19.7719
2100	471.426	702.128	1042.930	708.583	757.315	43.765	−19.7185
2200	474.242	749.414	1064.927	724.284	804.601	44.785	−19.6683
2300	476.750	796.966	1086.064	739.557	852.153	45.742	−19.6216
2400	478.991	844.755	1106.403	754.422	899.942	46.610	−19.5783
2500	481.000	892.756	1125.998	768.895	947.943	47.359	−19.5370
2600	482.808	940.948	1144.899	782.995	996.135	48.023	−19.4985
2700	484.440	989.312	1163.151	796.739	1044.499	48.559	−19.4629
2800	485.917	1037.831	1180.796	810.142	1093.018	48.977	−19.4295
2900	487.259	1086.491	1197.871	823.219	1141.678	49.268	−19.3974
3000	488.479	1135.279	1214.411	835.985	1190.466	49.402	−19.3673
3100	489.594	1184.183	1230.447	848.452	1239.370	49.438	−19.3402
3200	490.613	1233.195	1246.007	860.634	1288.381	49.311	−19.3141
3300	491.548	1282.303	1261.119	872.542	1337.490	49.044	−19.2897
3400	492.407	1331.502	1275.806	884.188	1386.689	48.634	−19.2668
3500	493.199	1380.783	1290.091	895.582	1435.969	48.058	−19.2459
3600	493.929	1430.139	1303.995	906.734	1485.326	47.348	−19.2258
3700	494.605	1479.567	1317.538	917.655	1534.754	46.469	−19.2077
3800	495.231	1529.059	1330.736	928.352	1584.246	45.435	−19.1902
3900	495.812	1578.611	1343.608	938.836	1633.798	44.250	−19.1748
4000	496.352	1628.220	1356.167	949.113	1683.407	42.876	−19.1597
4100	496.855	1677.880	1368.430	959.191	1733.067	41.372	−19.1469
4200	497.324	1727.590	1380.409	969.078	1782.777	39.689	−19.1346
4300	497.763	1777.344	1392.116	978.780	1832.531	37.828	−19.1229
4400	498.173	1827.141	1403.564	988.305	1882.328	35.763	−19.1122
4500	498.557	1876.978	1414.764	997.658	1932.165	33.567	−19.1032
4600	498.917	1926.852	1425.726	1006.845	1982.039	31.210	−19.0949
4700	499.255	1976.761	1436.459	1015.872	2031.948	28.698	−19.0877
4800	499.573	2026.702	1446.974	1024.744	2081.889	26.024	−19.0818
4900	499.873	2076.675	1457.278	1033.466	2131.862	23.191	−19.0766
5000	500.155	2126.676	1467.379	1042.044	2181.863	20.077	−19.0713
5100	500.422	2176.705	1477.286	1050.481	2231.892	16.943	−19.0686
5200	500.673	2226.760	1487.006	1058.783	2281.947	13.570	−19.0654
5300	500.911	2276.839	1496.545	1066.953	2332.026	10.030	−19.0632
5400	501.137	2326.942	1505.910	1074.995	2382.129	6.328	−19.0618
5500	501.350	2377.066	1515.108	1082.914	2432.253	2.462	−19.0610
5600	501.553	2427.212	1524.143	1090.713	2482.399	−1.569	−19.0608
5700	501.745	2477.377	1533.022	1098.395	2532.564	−5.757	−19.0615
5800	501.927	2527.560	1541.750	1105.964	2582.747	−10.104	−19.0628
5900	502.101	2577.762	1550.332	1113.423	2632.949	−14.607	−19.0646
6000	502.266	2627.980	1558.772	1120.775	2683.167	−19.259	−19.0671

TABLE 63. Molecular properties of $C_{12}H_8O_2$ (dibenzo-*p*-dioxin). Values listed with bold characters were chosen for thermodynamic calculations—$\sigma = \mathbf{4}$ and statistical weight = **1**

		Enthalpy of formation $\Delta_f H°(298.15\ \text{K})$ / kcal mol^{-1}			Zero point energy ZPE / kcal mol^{-1}	
Dorofeeva[39]		**−14.15±0.9**				
PM3		−7.95			105.399	
		Moments of inertia of the molecule / g cm^2×10^{-39}				
MOPAC method		I_a		I_b		I_c
Dorofeeva[25]		**39.2555**		**176.1272**		**215.3827**
PM3		39.6887		175.8305		215.4037
		Molecular vibrations / cm^{-1}				
Dorofeeva[25]	50.96	**114.7**	**219**	**246.5**	**254.5**	**298**
	373	**436**	**455**	**457**	**459**	**478**
	547	**583**	**645**	**653**	**689**	**690**
	727(2)*	**737**	**829**	**842**	**847**	**859**
	873	**953**	**954**	**1008(2)**	**1019**	**1031**
	1112	**1136**	**1171**	**1172**	**1222**	**1245**
	1263	**1293**	**1310**	**1316**	**1399**	**1407**
	1429	**1438**	**1502**	**1505**	**1572**	**1586**
	1593	**1634**	**3051(4)**	**3053(4)**		
PM3	42.5	119.7	188.5	241	255	275
	427	427	428	430	498	499
	542	615	627	698	700	715
	800(2)	841	882	893	904	907
	962	972	973	1014(2)	1112	1114
	1124	1135	1162	1164	1213	1224
	1265	1297	1345	1345	1398	1406
	1547	1577	1610	1644	1745	1765
	1781	1797	3024(4)	3036(2)	3049(2)	

*Numbers in parenthesis show multiplicity.

TABLE 64. Thermodynamic properties of $C_{12}H_8O_2$ (dibenzo-*p*-dioxin) (M_r = 184.194)

Enthalpy Reference Temperature = T_r = 298.15 K				Standard State Pressure = $p°$ = 0.1 MPa			
T (K)	C_p° (J·K^{-1}·mol^{-1})	$H°-H°(T_r)$ (J·mol^{-1})	$S°$ (J·K^{-1}·mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}·mol^{-1})	$H(T)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	log K_f
0	—	−28.336	—	—	−87.536	−32.342	—
100	64.413	−23.719	277.226	514.419	−82.919	−43.359	6.4414
200	119.052	−14.672	337.771	411.130	−73.872	−51.922	−5.7798
298.15	180.004	0.000	396.647	396.647	−59.200	−59.200	−10.5238
300	181.140	0.334	397.764	396.650	−58.866	−59.323	−10.5878
400	238.792	21.400	457.969	404.468	−37.800	−65.130	−13.2901
500	286.745	47.763	516.597	421.071	−11.437	−69.437	−15.0463
600	325.024	78.425	572.394	441.686	19.225	−72.580	−16.2820
700	355.512	112.508	624.873	464.147	53.308	−74.773	−17.1984
800	380.094	149.331	674.007	487.343	90.131	−76.155	−17.9029
900	400.197	188.378	719.975	510.665	129.178	−76.825	−18.4581
1000	416.840	229.256	763.028	533.772	170.056	−76.915	−18.9042
1100	430.753	271.655	803.429	556.469	212.455	−76.510	−19.2689
1200	442.478	315.333	841.426	578.648	256.133	−75.706	−19.5700
1300	452.425	360.092	877.247	600.253	300.892	−74.593	−19.8223
1400	460.917	405.770	911.094	621.258	346.570	−73.266	−20.0339
1500	468.206	452.235	943.149	641.658	393.035	−71.752	−20.2151
1600	474.496	499.378	973.572	661.460	440.178	−70.132	−20.3699
1700	479.952	547.107	1002.505	680.678	487.907	−68.453	−20.5028
1800	484.706	595.345	1030.076	699.329	536.145	−66.742	−20.6182
1900	488.870	644.028	1056.397	717.435	584.828	−65.038	−20.7189
2000	492.531	693.102	1081.568	735.017	633.902	−63.358	−20.8066
2100	495.765	742.520	1105.678	752.097	683.320	−61.726	−20.8848
2200	498.632	792.243	1128.809	768.698	733.043	−60.177	−20.9535
2300	501.185	842.236	1151.031	784.842	783.036	−58.696	−21.0149
2400	503.466	892.471	1172.410	800.548	833.271	−57.311	−21.0703
2500	505.511	942.921	1193.005	815.837	883.721	−56.055	−21.1192
2600	507.350	993.566	1212.868	830.727	934.366	−54.890	−21.1636
2700	509.011	1044.385	1232.047	845.238	985.185	−53.860	−21.2044
2800	510.513	1095.363	1250.586	859.385	1036.163	−52.958	−21.2416
2900	511.877	1146.483	1268.525	873.186	1087.283	−52.190	−21.2749
3000	513.119	1197.734	1285.900	886.655	1138.534	−51.587	−21.3055
3100	514.252	1249.104	1302.744	899.807	1189.904	−51.090	−21.3351
3200	515.289	1300.581	1319.087	912.655	1241.381	−50.765	−21.3618
3300	516.239	1352.158	1334.958	925.213	1292.958	−50.587	−21.3867
3400	517.113	1403.827	1350.383	937.492	1344.627	−50.560	−21.4101
3500	517.918	1455.579	1365.384	949.505	1396.379	−50.706	−21.4327
3600	518.660	1507.408	1379.985	961.260	1448.208	−50.993	−21.4535
3700	519.347	1559.309	1394.205	972.770	1500.109	−51.456	−21.4738
3800	519.983	1611.276	1408.064	984.044	1552.076	−52.081	−21.4927
3900	520.574	1663.304	1421.578	995.090	1604.104	−52.866	−21.5115
4000	521.123	1715.389	1434.765	1005.918	1656.189	−53.844	−21.5289
4100	521.634	1767.527	1447.639	1016.535	1708.327	−54.960	−21.5468
4200	522.111	1819.715	1460.215	1026.950	1760.515	−56.260	−21.5637
4300	522.556	1871.948	1472.506	1037.169	1812.748	−57.745	−21.5797
4400	522.973	1924.225	1484.524	1047.200	1865.025	−59.440	−21.5953
4500	523.363	1976.542	1496.281	1057.050	1917.342	−61.272	−21.6114
4600	523.729	2028.897	1507.788	1066.724	1969.697	−63.271	−21.6270
4700	524.073	2081.287	1519.055	1076.228	2022.087	−65.431	−21.6426
4800	524.396	2133.711	1530.092	1085.569	2074.511	−67.758	−21.6584
4900	524.701	2186.166	1540.908	1094.752	2126.966	−70.250	−21.6740
5000	524.988	2238.650	1551.512	1103.782	2179.450	−73.027	−21.6886
5100	525.258	2291.163	1561.910	1112.663	2231.963	−75.831	−21.7049
5200	525.514	2343.702	1572.112	1121.401	2284.502	−78.878	−21.7200
5300	525.756	2396.265	1582.125	1129.999	2337.065	−82.097	−21.7352
5400	525.985	2448.852	1591.954	1138.463	2389.652	−85.484	−21.7506
5500	526.202	2501.462	1601.608	1146.797	2442.262	−89.038	−21.7659
5600	526.407	2554.092	1611.091	1155.003	2494.892	−92.761	−21.7813
5700	526.603	2606.743	1620.410	1163.087	2547.543	−96.647	−21.7969
5800	526.788	2659.412	1629.570	1171.051	2600.212	−100.695	−21.8125
5900	526.964	2712.100	1638.577	1178.899	2652.900	−104.903	−21.8281
6000	527.132	2764.805	1647.435	1186.634	2705.605	−109.264	−21.8439

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