Thermodynamic Properties of Polybrominated/chlorinated Dibenzo-*p*-dioxins Calculated by Density Functional Theory

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Heat capacities, standard enthalpies of formation and entropies for 339 polybrominated/chlorinated dibenzo-*p*-dioxins (PXDDs) in the gas state were calculated using the density functional theory to construct a consistent set of thermodynamic values. The heat capacities and the entropies for PXDDs increase with increase in the substitute number of bromine and chlorine. As the degree of bromination increases, the standard enthalpies of formation and the Gibbs free energies of formation of PXDDs increase, while the degree of chlorination has only a small effect on their values compared with bromination. A much higher bromine potential than chlorine potential is needed for the formation of brominated dioxin congeners. However, the bromine-chlorine equilibrium potential for the formation of PXDDs suggested thermodynamically the possibility of their priority formation under the usual gaseous conditions where HBr and HCl are similar levels, because the bromine potential of the gas is much higher than the chlorine potential when the partial pressure of the two is similar.

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1. Introduction

Brominated flame retardants (BFRs) including tetra-bromobisphenol A (TBBPA), polybrominated diphenyl ethers (PBDEs), polybrominated biphenyls (PBBs), and hexabromocyclodecane (HBCD) have been widely used in plastics, textiles, electronic circuitry and other materials to prevent fires, and hold an important market share. Recycling activities for these consumer products containing BFRs are increasing and have become more important in recent years, due to the formation of polybrominated dibenzo-*p*-dioxins and furans (PBDD/Fs), and also mixed halogenated congeners such as polybrominated/chlorinated dibenzo-*p*-dioxins and furans (PXDD/Fs) in the case of thermal stress, because BFRs appear to be a main source of these brominated dioxin congeners in incinerators.¹⁻⁹⁾ However, the formation behaviors of brominated dioxin congeners from the incinerators have not yet been clarified, one of the reasons is that the current analytical methods are able to detect but not quantify all mixed brominated/chlorinated congeners. Because of the complexity of analytical procedures and lack of reference standards, it has been possible to characterize and determine only a small number of PBDD/F and PXDD/F isomers.

There is much less information on PBDD/Fs and PXDD/Fs than on their chlorinated analogues, and very little experimental data on their physicochemical properties. Using the thermodynamic data of PBDD/Fs and PXDD/Fs, it is possible to predict thermodynamically their formation in combustion gas from incineration.

We recently reported the calculated heat capacities, standard enthalpies of formation and entropies for 76 polybrominated dibenzo-*p*-dioxins (PBDDs) and 136 polybrominated dibenzofurans (PBDFs) using the density functional theory (DFT).^{10,11)} In this study, the thermodynamic properties were calculated for 339 PXDDs in the gas state using the DFT method with the Gaussian 98 program,¹²⁾ in order to show part of a consistent set of thermodynamic values for PXDD/Fs available for thermodynamic evaluation and consideration of their formation and decomposition in the combustion processes.

2. Computational Methods

Becke's three-parameter hybrid function combined with the gradient-correlation function of Lee, Yang and Parr (LYP), denoted B3LYP, was employed in the theoretical computations using DFT. The detailed method of calculating thermodynamic properties of brominated dioxins was shown in our last articles.^{10,11)} Heat capacity (C_p) and entropy (S°) were directly calculated using DFT and were directly obtained from the output of Gaussian programs. The equations used for calculating the absolute entropy of molecules are as follows:^{13,14)}

$$S = S_{\text{trans}} + S_{\text{rot}} + S_{\text{vib}} \quad (1)$$

where S_{trans} , S_{rot} and S_{vib} are translational, rotational and vibrational entropy, respectively, which can be calculated by the following equations:

$$S_{\text{trans}} = R \left[\frac{3}{2} \ln \left(\frac{2\pi m k T}{h^2} \right) + \ln \frac{kT}{p} + \frac{5}{2} \right] \quad (2)$$

$$S_{\text{rot}} = R \left[\ln \frac{\pi^{1/2}}{\sigma_r} + \frac{1}{2} \ln \frac{T^3}{(h^2/8\pi^2 I_x k)(h^2/8\pi^2 I_y k)(h^2/8\pi^2 I_z k)} + \frac{3}{2} \right] \quad (3)$$

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Fig. 3 Most and least stable isomers within the monobrominated dioxin homologues on the basis of standard free energies of formation at 298 K.

increase with increase in the substitution numbers of bromine and chlorine as shown in Fig. 2. One reason is thought to be the change in molecular weight with the substitutions of bromine and chlorine.

Figure 3 shows the most and least stable isomers on the basis of standard Gibbs free energies of formation at 298 K within the mono-brominated dioxin homologues calculated in this study. It is obvious that the most stable isomer has no or a minimum number of adjacent chlorine and bromine atoms, whereas the least stable isomer has a maximum number of nearest chlorines and bromines because the intramolecular repulsion energies affect the stability of the molecule.

Using the regression method, the correlations of thermodynamic properties ($\Delta_f H^\circ$, $\Delta_f G^\circ$, S° and C_p) at 298 K with the substitution number of bromine (x) and chlorine (y) were obtained for PXDDs from the calculated results of each isomer in the table in Appendix. The thermodynamic properties of PXDDs correlate very well with the degree of bromination (x), the obtained correlations being as follows:

For PXDDs,

$$\Delta_f H^\circ(298 \text{ K}) = (43.44 \pm 0.29)x - (9.78 \pm 0.29)y - (96.06 \pm 1.28), \quad R^2=0.988 \quad (11)$$

$$\Delta_f G^\circ(298 \text{ K}) = (35.04 \pm 0.30)x - (4.44 \pm 0.30)y + (17.88 \pm 1.32), \quad R^2=0.979 \quad (12)$$

$$S^\circ(298 \text{ K}) = (39.10 \pm 0.07)x + (28.68 \pm 0.07)y + (414.62 \pm 0.30), \quad R^2=0.999 \quad (13)$$

$$C_p(298 \text{ K}) = (16.82 \pm 0.02)x + (15.77 \pm 0.02)y + (181.59 \pm 0.07), \quad R^2=0.9998 \quad (14)$$

where R^2 indicates the coefficient of determination for the regression analysis. All these formulas indicate that the substitution number of bromine (x) has much more effect on the thermodynamic properties of PXDDs than the substitution number of chlorine (y).

Figure 4 shows the Gibbs free energy changes ($\Delta_r G^\circ$) in the brominated and chlorinated reactions of DD to 2,3,7,8-tetrabrominated/chlorinated dibenzo-*p*-dioxins (2,3,7,8-TeXDDs) shown in eq. (6) in which $m+n=4$. The values of $\Delta_r G^\circ$ increase with increase in degree of bromination of TeXDDs. It is suggested thermodynamically that the formation of higher brominated PXDDs cannot occur as easily as the lower brominated PXDDs and PCDDs.

Figure 5 shows the bromine-chlorine equilibrium potential for the formation of 2,3,7,8-TeXDDs ($\text{Br}_m\text{Cl}_{(4-m)}\text{DD}$) from 2,3,7,8-TeCDD at 573 K, where these potentials are represented by the partial pressures of Br_2 and Cl_2 , respectively. The diagram is based on the bromination reaction of 2,3,7,8-TeCDD as shown in the following:

Fig. 4 Gibbs free energy changes in the brominated and chlorinated reactions of DD to 2,3,7,8-TeXDDs.

Fig. 5 Bromine-chlorine equilibrium potential for the formation of 2,3,7,8-TeXDDs from 2,3,7,8-TeCDD at 573 K.

$$\Delta_r G^\circ = -RT \ln K = -RT \ln \frac{P_{\text{Br}_m\text{Cl}_{(4-m)}\text{DD}}^{2/m} P_{\text{Cl}_2}}{P_{\text{TeCDD}}^{2/m} P_{\text{Br}_2}} \quad (16)$$

where K and P indicate the equilibrium constant of reaction and partial pressure, respectively. The diagram was drawn assuming $P_{\text{TeCDD}} = P_{\text{Br}_m\text{Cl}_{(4-m)}\text{DD}}$ in order to know easily the possibility of bromination of the chlorinated dioxin congeners thermodynamically. The diagram shows that each 2,3,7,8-TeXDD can be thermodynamically formed from 2,3,7,8-TeCDD at higher bromine potential than each solid line, respectively. The equilibrium potentials of bromine and chlorine for the relationship between the gaseous HCl and HBr at their several partial pressure ratios are also shown by dotted lines based on the following reaction:

$$\Delta_r G^\circ = -RT \ln K = -RT \ln \frac{P_{\text{HBr}}^{1/2} P_{\text{Cl}_2}}{P_{\text{HCl}}^{1/2} P_{\text{Br}_2}} \quad (18)$$

The priority formations for each 2,3,7,8-TeXDD and their relationship with the ratio of HBr to HCl can be distinguished and discussed using this diagram. For example, when the ratio of HBr to HCl is 0.3, 2,3-Br₇-7,8-Cl₂-DD is supposed to be more stable than 2,3,7,8-TeCDD thermodynamically. From the diagram, it is suggested that much higher bromine potential than chlorine potential is needed for the formation of brominated dioxin congeners. However, even in the formation region of 2,3,7,8-TeBDD, the partial pressure of HBr can be lower than that of HCl such as HBr/HCl = 0.5, because HBr has thermodynamically much less stability than HCl and the equilibrium of the reaction shown in eq. (17) shifts to the left. In other words, when the partial pressure of HBr is similar to that of HCl in the gas, the bromine potential of the gas is far higher than the chlorine potential. Although a detailed discussion on the formation of brominated dioxin congeners is difficult using Fig. 5 because of the simplified calculations, the diagram can suggest thermodynamically the possibility of their priority formation under the usual gaseous conditions where HBr and HCl are at similar levels.

Yazawa *et al.*¹⁶⁾ evaluated thermodynamically the formation and decomposition behavior of PCDD/Fs, and the effects of temperature and gas compositions on them in the C-H-O-Cl quaternary combustion gas assuming homogeneous gas equilibrium. They used the consistent set of thermodynamic data of PCDD/Fs estimated by Menad.^{17,18)} Actually, the formation and decomposition of dioxin congeners are supposed to proceed in the heterogeneous gas solid interface, and the kinetic effects are also important and effective on their formation. The thermodynamic prediction is not necessarily agreement with the practical quantitative analysis in the incinerators. However, the thermodynamic evaluations can show us the approximate trends of the effect of gas compositions and temperature on their formation and decomposition behaviors.^{16,19)} Thermodynamic evaluations are useful for the formation and decomposition of dioxin congeners even for PCDD/Fs, because it is very difficult to clarify their complicated formation mechanism kinetically at present. There is much less information and fewer reports on the formation and decomposition behaviors of PBDD/Fs and PXDD/Fs in incinerators compared with PCDD/Fs, because of analytical difficulties. Using the consistent set of thermodynamic data for PBDD/Fs and PXDD/Fs, the thermodynamic evaluations and considerations would be possible for the brominated dioxin congeners in the combustion gas, and would provide important knowledge of their formation and decomposition behaviors.

4. Conclusion

The thermodynamic properties of 339 PXDDs in the gas state were calculated using the density functional theory (DFT) to construct a consistent set of thermodynamic values for them. As the degree of bromination increases, the standard enthalpies of formation for PXDD/Fs and the Gibbs free energies of formation of PXDDs increase, while the degree of chlorination has only a small effect on their values compared with bromination.

Much higher bromine potential than chlorine potential is needed for the formation of brominated dioxin congeners. However, the bromine-chlorine equilibrium potential for the formation of PXDDs suggested thermodynamically the possibility of their priority formation under the usual gaseous conditions where HBr and HCl are at similar levels, because the bromine potential of the gas is much higher than the chlorine potential when the partial pressure of the two is similar in the combustion gas.

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Appendix

Table A-1 Evaluated thermodynamic properties of gaseous PXDDs from 298.15 K to 1500 K at 101.325 kPa.

Compound	$\Delta_f H^\circ$ (298 K)	$\Delta_f G^\circ$ (298 K)	S° (298 K)	C_p , J·mol ⁻¹ ·K ⁻¹			
	kJ·mol ⁻¹	kJ·mol ⁻¹	J·mol ⁻¹ ·K ⁻¹	$C_p = A T^3 + B T^2 + C T + D$			
				A × 10 ⁷	B × 10 ⁴	C × 10	D
DD	-59.2 ^a	56.2	409.9	1.679	-6.610	9.596	-49.10
1-Br ₁ -2-Cl ₁ -DD	-45.0	66.8	479.3	1.682	-6.539	9.270	-6.906
1-Br ₁ -3-Cl ₁ -DD	-53.1	57.9	481.8	1.679	-6.526	9.251	-6.022
1-Br ₁ -4-Cl ₁ -DD	-46.4	64.6	482.1	1.676	-6.520	9.252	-6.533
1-Br ₁ -6-Cl ₁ -DD	-47.9	63.2	481.5	1.677	-6.523	9.254	-6.567
1-Br ₁ -7-Cl ₁ -DD	-55.4	55.9	480.9	1.681	-6.532	9.256	-6.193
1-Br ₁ -8-Cl ₁ -DD	-55.2	56.2	480.9	1.681	-6.532	9.257	-6.210
1-Br ₁ -9-Cl ₁ -DD	-46.4	65.1	480.3	1.678	-6.526	9.257	-6.656
2-Br ₁ -1-Cl ₁ -DD	-43.4	68.1	480.2	1.679	-6.529	9.259	-6.534
2-Br ₁ -3-Cl ₁ -DD	-50.6	60.9	480.3	1.682	-6.534	9.258	-6.083
2-Br ₁ -4-Cl ₁ -DD	-51.3	59.7	482.0	1.676	-6.516	9.240	-5.583
2-Br ₁ -6-Cl ₁ -DD	-53.5	57.5	481.9	1.678	-6.522	9.245	-5.675
2-Br ₁ -7-Cl ₁ -DD	-61.1	50.4	480.5	1.682	-6.533	9.250	-5.530
2-Br ₁ -8-Cl ₁ -DD	-60.9	50.4	481.0	1.682	-6.532	9.249	-5.414
2-Br ₁ -9-Cl ₁ -DD	-53.2	57.8	481.9	1.678	-6.523	9.245	-5.683
1-Br ₁ -2,3-Cl ₂ -DD	-58.6	58.5	508.2	1.691	-6.528	9.134	13.13
1-Br ₁ -2,4-Cl ₂ -DD	-62.0	54.4	510.3	1.685	-6.510	9.118	13.50
1-Br ₁ -2,6-Cl ₂ -DD	-65.7	50.6	510.8	1.689	-6.519	9.123	13.52
1-Br ₁ -2,7-Cl ₂ -DD	-73.1	43.5	509.7	1.693	-6.529	9.128	13.76
1-Br ₁ -2,8-Cl ₂ -DD	-72.9	43.5	510.5	1.693	-6.529	9.127	13.83
1-Br ₁ -2,9-Cl ₂ -DD	-64.2	52.5	509.5	1.690	-6.523	9.128	13.31
1-Br ₁ -3,4-Cl ₂ -DD	-60.7	55.7	510.6	1.684	-6.507	9.117	13.37
1-Br ₁ -3,6-Cl ₂ -DD	-73.4	42.4	512.6	1.685	-6.506	9.107	14.17
1-Br ₁ -3,7-Cl ₂ -DD	-81.0	35.0	511.9	1.689	-6.515	9.109	14.60
1-Br ₁ -3,8-Cl ₂ -DD	-80.8	35.3	511.5	1.689	-6.516	9.111	14.52
1-Br ₁ -3,9-Cl ₂ -DD	-72.1	43.8	511.9	1.686	-6.509	9.109	14.13
1-Br ₁ -4,6-Cl ₂ -DD	-65.5	50.9	510.4	1.683	-6.502	9.110	13.60
1-Br ₁ -4,7-Cl ₂ -DD	-74.3	41.8	511.7	1.686	-6.510	9.111	14.05
1-Br ₁ -4,8-Cl ₂ -DD	-74.3	41.9	511.2	1.686	-6.510	9.112	13.95
1-Br ₁ -4,9-Cl ₂ -DD	-65.6	50.6	511.2	1.682	-6.500	9.109	13.60
1-Br ₁ -6,7-Cl ₂ -DD	-64.2	52.2	510.7	1.686	-6.513	9.120	13.42
1-Br ₁ -6,8-Cl ₂ -DD	-73.0	43.1	511.5	1.685	-6.505	9.106	14.14
1-Br ₁ -6,9-Cl ₂ -DD	-65.4	50.6	511.7	1.681	-6.496	9.104	13.79
1-Br ₁ -7,8-Cl ₂ -DD	-71.1	45.6	509.8	1.689	-6.519	9.120	13.37
1-Br ₁ -7,9-Cl ₂ -DD	-71.8	44.1	512.2	1.685	-6.506	9.106	14.21

continued on the next page

Compound	$\Delta_f H^\circ$ (298 K)	$\Delta_f G^\circ$ (298 K)	S° (298 K)	$C_p, \text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$			
	$\text{kJ}\cdot\text{mol}^{-1}$	$\text{kJ}\cdot\text{mol}^{-1}$	$\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$	$C_p = A T^3 + B T^2 + C T + D$			
				$A \times 10^7$	$B \times 10^4$	$C \times 10$	D
1-Br ₁ -8,9-Cl ₂ -DD	-62.6	54.0	509.9	1.687	-6.517	9.124	13.28
2-Br ₁ -1,3-Cl ₂ -DD	-58.3	58.8	508.2	1.690	-6.523	9.128	13.40
2-Br ₁ -1,4-Cl ₂ -DD	-60.6	56.1	509.5	1.682	-6.500	9.108	13.76
2-Br ₁ -1,6-Cl ₂ -DD	-64.0	52.4	510.5	1.686	-6.511	9.116	13.67
2-Br ₁ -1,7-Cl ₂ -DD	-71.4	45.0	510.4	1.690	-6.521	9.119	14.04
2-Br ₁ -1,8-Cl ₂ -DD	-71.2	45.2	510.7	1.690	-6.520	9.118	14.10
2-Br ₁ -1,9-Cl ₂ -DD	-62.3	54.3	509.9	1.687	-6.513	9.119	13.56
2-Br ₁ -3,4-Cl ₂ -DD	-57.0	60.3	507.7	1.689	-6.521	9.127	13.37
2-Br ₁ -3,6-Cl ₂ -DD	-71.0	45.5	510.1	1.689	-6.517	9.117	14.04
2-Br ₁ -3,7-Cl ₂ -DD	-78.4	38.0	510.6	1.692	-6.525	9.118	14.49
2-Br ₁ -3,8-Cl ₂ -DD	-78.6	37.9	510.4	1.692	-6.524	9.117	14.54
2-Br ₁ -3,9-Cl ₂ -DD	-71.0	46.0	508.7	1.689	-6.519	9.119	13.92
2-Br ₁ -4,6-Cl ₂ -DD	-70.0	45.8	512.5	1.683	-6.499	9.098	14.66
2-Br ₁ -4,7-Cl ₂ -DD	-78.9	37.2	511.7	1.687	-6.506	9.099	14.96
2-Br ₁ -4,8-Cl ₂ -DD	-79.0	36.7	512.8	1.686	-6.506	9.098	15.08
2-Br ₁ -4,9-Cl ₂ -DD	-71.6	44.4	512.1	1.683	-6.497	9.096	14.64
2-Br ₁ -6,7-Cl ₂ -DD	-69.5	46.5	511.9	1.688	-6.514	9.112	14.28
2-Br ₁ -6,8-Cl ₂ -DD	-78.7	37.3	511.9	1.686	-6.504	9.097	15.01
2-Br ₁ -6,9-Cl ₂ -DD	-72.1	43.7	512.6	1.674	-6.470	9.071	15.37
2-Br ₁ -7,8-Cl ₂ -DD	-76.7	39.5	511.3	1.690	-6.517	9.111	14.65
2-Br ₁ -7,9-Cl ₂ -DD	-78.5	37.5	511.7	1.686	-6.505	9.099	14.95
2-Br ₁ -8,9-Cl ₂ -DD	-69.2	47.2	510.5	1.688	-6.514	9.113	14.19
1-Br ₁ -2,3,4-Cl ₃ -DD	-63.1	59.5	536.6	1.698	-6.514	9.003	32.55
1-Br ₁ -2,3,7-Cl ₃ -DD	-85.9	36.0	538.5	1.702	-6.520	8.995	33.72
1-Br ₁ -2,3,9-Cl ₃ -DD	-77.2	44.6	539.1	1.699	-6.512	8.993	33.38
1-Br ₁ -2,4,6-Cl ₃ -DD	-80.6	40.8	540.2	1.692	-6.492	8.975	33.68
1-Br ₁ -2,4,8-Cl ₃ -DD	-89.2	32.1	540.7	1.696	-6.501	8.978	34.07
1-Br ₁ -2,6,7-Cl ₃ -DD	-81.4	40.2	539.7	1.699	-6.511	8.992	33.35
1-Br ₁ -2,6,9-Cl ₃ -DD	-82.7	38.5	541.1	1.693	-6.495	8.976	33.77
1-Br ₁ -2,7,8-Cl ₃ -DD	-88.3	33.6	538.5	1.702	-6.518	8.993	33.66
1-Br ₁ -2,8,9-Cl ₃ -DD	-79.9	42.2	538.1	1.700	-6.515	8.996	33.18
1-Br ₁ -3,4,8-Cl ₃ -DD	-87.8	33.4	541.0	1.695	-6.498	8.978	33.85
1-Br ₁ -3,4,9-Cl ₃ -DD	-79.4	41.7	541.4	1.691	-6.489	8.974	33.57
1-Br ₁ -3,6,8-Cl ₃ -DD	-97.7	22.9	542.9	1.693	-6.489	8.960	34.92
1-Br ₁ -3,7,9-Cl ₃ -DD	-96.8	24.2	541.8	1.694	-6.491	8.963	34.77
1-Br ₁ -4,6,7-Cl ₃ -DD	-81.0	40.3	540.6	1.692	-6.493	8.978	33.51
1-Br ₁ -4,7,8-Cl ₃ -DD	-89.3	31.9	540.9	1.695	-6.497	8.976	33.95
1-Br ₁ -6,7,8-Cl ₃ -DD	-76.5	45.1	539.6	1.695	-6.502	8.987	33.27
1-Br ₁ -6,7,9-Cl ₃ -DD	-78.8	42.4	540.7	1.689	-6.482	8.968	33.68
2-Br ₁ -1,3,4-Cl ₃ -DD	-62.6	59.3	538.6	1.696	-6.506	8.994	32.99
2-Br ₁ -1,3,6-Cl ₃ -DD	-78.2	43.9	538.2	1.697	-6.505	8.986	33.64
2-Br ₁ -1,3,8-Cl ₃ -DD	-85.5	36.3	539.1	1.701	-6.515	8.989	33.99
2-Br ₁ -1,4,6-Cl ₃ -DD	-79.1	42.1	541.0	1.689	-6.480	8.963	34.06
2-Br ₁ -1,4,7-Cl ₃ -DD	-87.6	33.5	541.3	1.693	-6.490	8.966	34.45
2-Br ₁ -1,4,9-Cl ₃ -DD	-79.0	42.2	540.9	1.702	-6.522	9.005	32.73
2-Br ₁ -1,6,8-Cl ₃ -DD	-88.6	32.5	541.5	1.694	-6.493	8.968	34.44
2-Br ₁ -1,7,8-Cl ₃ -DD	-86.5	35.1	539.6	1.699	-6.508	8.984	33.99
2-Br ₁ -1,8,9-Cl ₃ -DD	-77.9	43.4	540.8	1.697	-6.505	8.985	33.64
2-Br ₁ -3,4,7-Cl ₃ -DD	-83.9	37.9	539.0	1.700	-6.512	8.987	33.94
2-Br ₁ -3,4,9-Cl ₃ -DD	-76.7	45.1	538.9	1.695	-6.501	8.982	33.65
2-Br ₁ -3,6,7-Cl ₃ -DD	-86.5	35.3	539.0	1.699	-6.510	8.985	33.96
2-Br ₁ -3,6,9-Cl ₃ -DD	-89.1	32.2	540.6	1.693	-6.491	8.967	34.43
2-Br ₁ -3,7,8-Cl ₃ -DD	-93.8	27.9	539.4	1.701	-6.513	8.982	34.43
2-Br ₁ -3,8,9-Cl ₃ -DD	-86.4	35.4	538.9	1.699	-6.509	8.985	33.96
2-Br ₁ -4,6,8-Cl ₃ -DD	-94.8	26.4	540.9	1.692	-6.484	8.955	35.11

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Compound	$\Delta_f H^\circ$ (298 K)	$\Delta_f G^\circ$ (298 K)	S° (298 K)	$C_p, \text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$			
	$\text{kJ}\cdot\text{mol}^{-1}$	$\text{kJ}\cdot\text{mol}^{-1}$	$\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$	$C_p = A T^3 + B T^2 + C T + D$			
				$A \times 10^7$	$B \times 10^4$	$C \times 10$	D
2-Br ₁ -4,7,8-Cl ₃ -DD	-94.0	27.0	541.9	1.695	-6.494	8.964	34.97
2-Br ₁ -4,8,9-Cl ₃ -DD	-87.0	34.1	541.5	1.693	-6.489	8.965	34.51
2-Br ₁ -6,7,8-Cl ₃ -DD	-82.1	39.5	539.5	1.697	-6.505	8.978	34.16
2-Br ₁ -6,8,9-Cl ₃ -DD	-85.3	35.5	542.1	1.690	-6.482	8.958	34.66
1-Br ₁ -2,3,4,6-Cl ₄ -DD	-81.0	46.1	567.8	1.705	-6.496	8.862	52.76
1-Br ₁ -2,3,4,8-Cl ₄ -DD	-89.7	37.7	566.9	1.709	-6.506	8.865	53.02
1-Br ₁ -2,3,6,8-Cl ₄ -DD	-102.5	24.1	569.5	1.706	-6.494	8.845	54.10
1-Br ₁ -2,3,7,8-Cl ₄ -DD	-100.6	26.5	567.6	1.712	-6.510	8.862	53.64
1-Br ₁ -2,3,8,9-Cl ₄ -DD	-92.4	34.7	567.7	1.709	-6.504	8.862	53.26
1-Br ₁ -2,4,6,8-Cl ₄ -DD	-104.6	21.6	570.9	1.700	-6.474	8.828	54.40
1-Br ₁ -2,4,7,8-Cl ₄ -DD	-103.9	22.8	569.2	1.705	-6.491	8.845	53.94
1-Br ₁ -2,4,8,9-Cl ₄ -DD	-95.7	30.5	570.7	1.702	-6.484	8.844	53.55
1-Br ₁ -2,6,7,9-Cl ₄ -DD	-95.8	30.9	569.2	1.701	-6.481	8.841	53.64
1-Br ₁ -2,7,8,9-Cl ₄ -DD	-92.2	34.8	568.4	1.708	-6.503	8.860	53.27
1-Br ₁ -3,4,6,8-Cl ₄ -DD	-103.0	23.1	570.9	1.699	-6.473	8.829	54.23
1-Br ₁ -3,4,7,8-Cl ₄ -DD	-102.5	24.1	569.4	1.704	-6.487	8.843	53.79
1-Br ₁ -3,4,8,9-Cl ₄ -DD	-94.5	31.9	570.4	1.701	-6.482	8.843	53.41
1-Br ₁ -3,6,7,9-Cl ₄ -DD	-103.1	23.1	570.9	1.697	-6.467	8.824	54.37
1-Br ₁ -3,7,8,9-Cl ₄ -DD	-99.9	26.8	569.4	1.705	-6.491	8.845	53.85
1-Br ₁ -4,6,7,9-Cl ₄ -DD	-95.2	30.9	571.2	1.694	-6.461	8.824	53.89
1-Br ₁ -4,7,8,9-Cl ₄ -DD	-93.2	33.3	569.9	1.701	-6.483	8.843	53.48
1-Br ₁ -6,7,8,9-Cl ₄ -DD	-79.2	47.8	568.2	1.700	-6.484	8.853	52.76
2-Br ₁ -1,3,4,7-Cl ₄ -DD	-89.3	38.0	567.4	1.707	-6.500	8.857	53.43
2-Br ₁ -1,3,4,9-Cl ₄ -DD	-80.7	46.3	568.4	1.703	-6.489	8.852	53.20
2-Br ₁ -1,3,6,7-Cl ₄ -DD	-93.3	33.7	568.1	1.707	-6.499	8.855	53.49
2-Br ₁ -1,3,6,9-Cl ₄ -DD	-94.4	32.4	568.9	1.702	-6.483	8.841	53.84
2-Br ₁ -1,3,7,8-Cl ₄ -DD	-100.3	27.1	567.0	1.710	-6.505	8.856	53.85
2-Br ₁ -1,4,6,7-Cl ₄ -DD	-94.2	32.1	570.5	1.699	-6.474	8.833	53.94
2-Br ₁ -1,4,6,9-Cl ₄ -DD	-95.3	30.8	571.1	1.693	-6.456	8.816	54.30
2-Br ₁ -1,4,7,9-Cl ₄ -DD	-102.8	23.4	570.9	1.697	-6.465	8.819	54.67
2-Br ₁ -1,6,7,8-Cl ₄ -DD	-91.8	35.1	568.6	1.705	-6.492	8.850	53.51
2-Br ₁ -1,6,8,9-Cl ₄ -DD	-93.7	32.7	570.4	1.698	-6.472	8.831	53.96
2-Br ₁ -3,4,6,8-Cl ₄ -DD	-99.5	27.3	569.0	1.704	-6.487	8.839	54.29
2-Br ₁ -3,4,7,8-Cl ₄ -DD	-98.9	28.0	568.3	1.709	-6.501	8.852	53.93
2-Br ₁ -3,4,8,9-Cl ₄ -DD	-92.0	34.9	568.6	1.706	-6.494	8.851	53.59
2-Br ₁ -3,6,7,8-Cl ₄ -DD	-98.6	28.3	568.3	1.708	-6.499	8.850	53.95
2-Br ₁ -3,7,8,9-Cl ₄ -DD	-98.7	28.5	567.5	1.708	-6.499	8.852	53.83
2-Br ₁ -4,6,7,8-Cl ₄ -DD	-97.7	28.9	569.6	1.703	-6.483	8.835	54.30
2-Br ₁ -4,6,8,9-Cl ₄ -DD	-101.0	25.1	571.3	1.695	-6.458	8.812	54.87
2-Br ₁ -6,7,8,9-Cl ₄ -DD	-85.7	41.3	568.1	1.703	-6.486	8.847	53.53
1-Br ₁ -2,3,4,6,8-Cl ₅ -DD	-104.7	27.1	598.7	1.713	-6.480	8.716	73.43
1-Br ₁ -2,3,4,7,8-Cl ₅ -DD	-104.0	28.6	596.0	1.718	-6.496	8.732	72.90
1-Br ₁ -2,3,4,8,9-Cl ₅ -DD	-96.1	36.2	596.8	1.716	-6.491	8.732	72.57
1-Br ₁ -2,3,6,7,8-Cl ₅ -DD	-105.3	27.0	596.8	1.717	-6.493	8.727	73.21
1-Br ₁ -2,3,6,7,9-Cl ₅ -DD	-107.6	24.3	598.4	1.711	-6.472	8.708	73.62
1-Br ₁ -2,3,7,8,9-Cl ₅ -DD	-104.3	28.2	596.1	1.718	-6.495	8.730	73.05
1-Br ₁ -2,4,6,7,9-Cl ₅ -DD	-109.6	21.6	600.5	1.704	-6.453	8.692	73.91
1-Br ₁ -2,4,7,8,9-Cl ₅ -DD	-107.5	24.6	597.5	1.712	-6.476	8.712	73.40
1-Br ₁ -3,4,6,7,8-Cl ₅ -DD	-105.9	26.1	597.8	1.710	-6.473	8.712	73.26
1-Br ₁ -3,4,6,8,9-Cl ₅ -DD	-108.1	22.9	601.2	1.703	-6.450	8.690	73.79
1-Br ₁ -3,6,7,8,9-Cl ₅ -DD	-103.1	28.7	598.6	1.710	-6.472	8.710	73.38
1-Br ₁ -4,6,7,8,9-Cl ₅ -DD	-95.3	36.3	599.3	1.707	-6.465	8.710	72.86
2-Br ₁ -1,3,4,6,7-Cl ₅ -DD	-95.6	37.0	596.1	1.714	-6.484	8.725	72.90
2-Br ₁ -1,3,4,6,9-Cl ₅ -DD	-96.7	35.2	598.3	1.707	-6.465	8.705	73.44
2-Br ₁ -1,3,4,7,8-Cl ₅ -DD	-103.7	28.8	596.1	1.717	-6.490	8.725	73.31

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Compound	$\Delta_f H^\circ$ (298 K)	$\Delta_f G^\circ$ (298 K)	S° (298 K)	$C_p, \text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$			
	$\text{kJ}\cdot\text{mol}^{-1}$	$\text{kJ}\cdot\text{mol}^{-1}$	$\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$	$C_p = A T^3 + B T^2 + C T + D$			
				$A \times 10^7$	$B \times 10^4$	$C \times 10$	D
2-Br ₁ -1,3,6,7,8-Cl ₅ -DD	−105.0	27.4	596.6	1.716	−6.489	8.722	73.43
2-Br ₁ -1,3,6,8,9-Cl ₅ -DD	−106.9	25.0	598.2	1.710	−6.468	8.703	73.87
2-Br ₁ -1,3,7,8,9-Cl ₅ -DD	−103.7	28.7	596.6	1.717	−6.492	8.725	73.37
2-Br ₁ -1,4,7,8,9-Cl ₅ -DD	−105.6	26.5	597.9	1.708	−6.465	8.702	73.73
2-Br ₁ -3,4,6,7,8-Cl ₅ -DD	−102.3	30.3	596.1	1.716	−6.487	8.721	73.40
2-Br ₁ -3,4,7,8,9-Cl ₅ -DD	−103.6	28.7	597.2	1.715	−6.485	8.719	73.46
2-Br ₁ -3,6,7,8,9-Cl ₅ -DD	−101.8	30.6	596.5	1.714	−6.483	8.719	73.37
2-Br ₁ -4,6,7,8,9-Cl ₅ -DD	−101.0	30.8	598.7	1.707	−6.462	8.698	73.91
1-Br ₁ -2,3,4,6,7,8-Cl ₆ -DD	−107.2	30.5	625.5	1.725	−6.482	8.600	92.45
1-Br ₁ -2,3,4,7,8,9-Cl ₆ -DD	−107.5	30.4	624.8	1.725	−6.481	8.600	92.40
1-Br ₁ -2,3,6,7,8,9-Cl ₆ -DD	−107.4	30.5	624.8	1.723	−6.477	8.596	92.57
1-Br ₁ -3,4,6,7,8,9-Cl ₆ -DD	−107.9	29.4	627.0	1.716	−6.455	8.578	92.75
2-Br ₁ -1,3,4,6,7,8-Cl ₆ -DD	−107.0	31.3	623.6	1.724	−6.477	8.595	92.68
2-Br ₁ -1,3,4,7,8,9-Cl ₆ -DD	−106.8	31.2	624.4	1.723	−6.475	8.592	92.83
2-Br ₁ -1,3,6,7,8,9-Cl ₆ -DD	−106.8	31.0	625.3	1.723	−6.474	8.591	92.84
2-Br ₁ -3,4,6,7,8,9-Cl ₆ -DD	−105.3	32.2	626.1	1.721	−6.469	8.587	92.89
1-Br ₁ -2,3,4,6,7,8,9-Cl ₇ -DD	−109.2	33.8	654.3	1.730	−6.464	8.467	111.9
2-Br ₁ -1,3,4,6,7,8,9-Cl ₇ -DD	−108.5	34.4	654.5	1.729	−6.458	8.459	112.3
1,2-Br ₂ -3-Cl ₁ -DD	−6.4	96.8	519.1	1.678	−6.482	9.080	15.54
1,3-Br ₂ -9-Cl ₁ -DD	−16.0	86.2	522.7	1.670	−6.454	9.048	16.58
1,4-Br ₂ -7-Cl ₁ -DD	−19.7	82.3	523.2	1.673	−6.466	9.064	15.84
1,6-Br ₂ -3-Cl ₁ -DD	−18.7	83.2	523.6	1.671	−6.460	9.057	16.10
1,7-Br ₂ -8-Cl ₁ -DD	−16.2	86.1	521.8	1.675	−6.471	9.065	16.08
1,8-Br ₂ -6-Cl ₁ -DD	−17.0	85.0	523.2	1.669	−6.451	9.045	16.64
1,9-Br ₂ -3-Cl ₁ -DD	−17.7	84.2	523.4	1.672	−6.463	9.059	16.03
2,3-Br ₂ -7-Cl ₁ -DD	−24.8	77.8	520.9	1.677	−6.474	9.060	16.79
2,7-Br ₂ -4-Cl ₁ -DD	−22.3	79.8	522.8	1.671	−6.454	9.041	17.29
2,8-Br ₂ -3-Cl ₁ -DD	−22.0	80.6	521.2	1.676	−6.470	9.056	16.89
1,2-Br ₂ -3,4-Cl ₂ -DD	−11.1	97.7	547.2	1.685	−6.469	8.951	34.84
1,3-Br ₂ -7,9-Cl ₂ -DD	−40.6	66.3	553.4	1.678	−6.437	8.901	37.28
1,4-Br ₂ -6,9-Cl ₂ -DD	−28.2	79.1	552.2	1.673	−6.430	8.911	35.81
1,6-Br ₂ -2,8-Cl ₂ -DD	−36.0	71.6	550.8	1.683	−6.458	8.929	36.02
1,7-Br ₂ -3,9-Cl ₂ -DD	−40.5	66.3	553.3	1.678	−6.438	8.902	37.22
1,8-Br ₂ -3,7-Cl ₂ -DD	−41.2	66.1	551.9	1.684	−6.455	8.919	36.84
1,9-Br ₂ -2,7-Cl ₂ -DD	−35.1	72.4	551.2	1.684	−6.460	8.930	36.03
2,3-Br ₂ -1,8-Cl ₂ -DD	−32.0	75.8	550.1	1.687	−6.466	8.933	36.36
2,3-Br ₂ -7,8-Cl ₂ -DD	−40.2	67.9	549.4	1.686	−6.463	8.927	36.62
2,7-Br ₂ -3,4-Cl ₂ -DD	−27.6	80.3	550.0	1.683	−6.456	8.924	36.47
2,7-Br ₂ -3,8-Cl ₂ -DD	−38.9	69.0	549.9	1.686	−6.464	8.926	36.24
2,8-Br ₂ -1,7-Cl ₂ -DD	−31.9	76.0	549.9	1.684	−6.460	8.929	36.24
2,8-Br ₂ -3,7-Cl ₂ -DD	−39.1	69.0	549.0	1.687	−6.467	8.930	36.53
1,2-Br ₂ -3,4,7-Cl ₃ -DD	−37.8	75.8	577.2	1.696	−6.463	8.813	55.38
1,2-Br ₂ -3,7,8-Cl ₃ -DD	−48.6	64.8	578.4	1.698	−6.464	8.808	55.95
1,2-Br ₂ -6,7,9-Cl ₃ -DD	−42.2	70.4	580.6	1.686	−6.429	8.783	55.93
1,3-Br ₂ -2,4,6-Cl ₃ -DD	−28.1	85.1	578.6	1.692	−6.452	8.809	55.08
1,3-Br ₂ -2,7,8-Cl ₃ -DD	−46.3	67.4	577.1	1.697	−6.462	8.807	55.86
1,3-Br ₂ -7,8,9-Cl ₃ -DD	−43.8	68.9	580.4	1.689	−6.436	8.783	56.38
1,4-Br ₂ -2,6,9-Cl ₃ -DD	−43.1	69.0	582.6	1.684	−6.425	8.782	55.64
1,4-Br ₂ -6,7,8-Cl ₃ -DD	−38.9	73.8	580.7	1.687	−6.437	8.793	55.40
1,6-Br ₂ -3,4,8-Cl ₃ -DD	−49.2	63.0	582.3	1.686	−6.428	8.779	56.20
1,7-Br ₂ -2,3,8-Cl ₃ -DD	−46.0	67.6	577.6	1.697	−6.462	8.808	55.80
1,7-Br ₂ -2,4,9-Cl ₃ -DD	−48.4	64.0	581.8	1.685	−6.423	8.771	56.72
1,7-Br ₂ -3,4,8-Cl ₃ -DD	−47.7	64.8	581.0	1.689	−6.439	8.788	56.10
1,8-Br ₂ -2,3,7-Cl ₃ -DD	−46.0	67.2	578.7	1.697	−6.461	8.805	55.96
1,8-Br ₂ -3,4,6-Cl ₃ -DD	−47.0	65.0	582.6	1.683	−6.419	8.769	56.63

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Compound	$\Delta_f H^\circ$ (298 K)	$\Delta_f G^\circ$ (298 K)	S° (298 K)	$C_p, \text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$			
	$\text{kJ}\cdot\text{mol}^{-1}$	$\text{kJ}\cdot\text{mol}^{-1}$	$\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$	$C_p = A T^3 + B T^2 + C T + D$			
				$A \times 10^7$	$B \times 10^4$	$C \times 10$	D
1,8-Br ₂ -6,7,9-Cl ₃ -DD	-26.3	87.4	577.0	1.689	-6.445	8.804	54.96
1,9-Br ₂ -2,4,7-Cl ₃ -DD	-50.7	61.5	581.9	1.687	-6.432	8.782	56.20
2,3-Br ₂ -1,7,8-Cl ₃ -DD	-46.7	66.6	578.4	1.696	-6.456	8.799	56.26
2,3-Br ₂ -6,7,8-Cl ₃ -DD	-45.0	68.8	576.8	1.694	-6.452	8.799	55.97
2,7-Br ₂ -1,3,8-Cl ₃ -DD	-45.6	67.7	578.3	1.696	-6.457	8.800	56.21
2,7-Br ₂ -3,4,8-Cl ₃ -DD	-44.1	69.3	578.0	1.695	-6.454	8.799	56.14
2,8-Br ₂ -1,3,7-Cl ₃ -DD	-45.6	67.8	578.3	1.696	-6.457	8.800	56.25
2,8-Br ₂ -3,4,7-Cl ₃ -DD	-44.2	69.1	578.6	1.694	-6.452	8.796	56.23
1,2-Br ₂ -3,4,7,8-Cl ₄ -DD	-52.1	66.5	607.0	1.706	-6.453	8.680	75.30
1,2-Br ₂ -3,6,7,8-Cl ₄ -DD	-53.4	65.5	606.2	1.704	-6.448	8.675	75.47
1,2-Br ₂ -3,7,8,9-Cl ₄ -DD	-52.4	66.4	606.6	1.705	-6.450	8.677	75.38
1,3-Br ₂ -2,4,7,8-Cl ₄ -DD	-51.4	67.3	606.9	1.706	-6.453	8.680	75.32
1,3-Br ₂ -2,6,7,8-Cl ₄ -DD	-51.2	67.9	605.7	1.704	-6.446	8.673	75.40
1,3-Br ₂ -2,7,8,9-Cl ₄ -DD	-50.0	68.6	607.1	1.704	-6.446	8.673	75.49
1,3-Br ₂ -4,7,8,9-Cl ₄ -DD	-52.1	66.2	608.3	1.696	-6.424	8.657	75.49
1,4-Br ₂ -2,3,7,8-Cl ₄ -DD	-51.5	67.3	606.6	1.707	-6.460	8.690	74.78
1,4-Br ₂ -6,7,8,9-Cl ₄ -DD	-41.2	76.7	609.9	1.693	-6.420	8.661	74.78
1,6-Br ₂ -2,3,7,8-Cl ₄ -DD	-51.5	67.3	606.6	1.707	-6.456	8.684	75.06
1,6-Br ₂ -2,4,7,9-Cl ₄ -DD	-57.2	60.6	610.0	1.694	-6.419	8.651	75.65
1,7-Br ₂ -2,3,4,8-Cl ₄ -DD	-49.4	69.4	606.8	1.704	-6.446	8.675	75.32
1,7-Br ₂ -2,3,6,8-Cl ₄ -DD	-52.4	66.6	606.0	1.706	-6.452	8.679	75.33
1,7-Br ₂ -2,3,8,9-Cl ₄ -DD	-50.0	68.6	607.3	1.704	-6.448	8.675	75.39
1,7-Br ₂ -3,4,8,9-Cl ₄ -DD	-51.8	66.2	609.2	1.697	-6.425	8.657	75.60
1,8-Br ₂ -2,3,4,7-Cl ₄ -DD	-49.2	69.6	606.5	1.704	-6.448	8.677	75.20
1,8-Br ₂ -2,3,6,7-Cl ₄ -DD	-50.9	67.9	606.7	1.704	-6.446	8.674	75.37
1,8-Br ₂ -2,3,7,9-Cl ₄ -DD	-51.4	67.3	607.0	1.706	-6.453	8.678	75.43
1,8-Br ₂ -2,4,7,9-Cl ₄ -DD	-54.6	64.0	607.6	1.699	-6.432	8.661	75.67
1,9-Br ₂ -2,3,7,8-Cl ₄ -DD	-52.2	66.6	606.5	1.706	-6.455	8.682	75.15
1,9-Br ₂ -2,4,6,8-Cl ₄ -DD	-57.6	60.2	610.1	1.693	-6.415	8.647	75.81
2,3-Br ₂ -1,4,7,8-Cl ₄ -DD	-51.9	67.3	605.4	1.704	-6.448	8.674	75.57
2,3-Br ₂ -1,6,7,8-Cl ₄ -DD	-51.6	67.3	606.4	1.702	-6.441	8.667	75.69
2,3-Br ₂ -1,7,8,9-Cl ₄ -DD	-50.4	68.6	606.1	1.703	-6.444	8.670	75.62
2,3-Br ₂ -6,7,8,9-Cl ₄ -DD	-48.2	70.9	605.5	1.699	-6.434	8.665	75.46
2,7-Br ₂ -1,3,4,8-Cl ₄ -DD	-48.9	69.8	606.8	1.702	-6.441	8.668	75.65
2,7-Br ₂ -1,3,6,8-Cl ₄ -DD	-52.1	67.0	605.9	1.705	-6.448	8.673	75.62
2,7-Br ₂ -1,3,8,9-Cl ₄ -DD	-49.5	69.6	605.8	1.704	-6.447	8.673	75.51
2,7-Br ₂ -3,4,8,9-Cl ₄ -DD	-49.0	69.6	607.1	1.701	-6.437	8.665	75.71
2,8-Br ₂ -1,3,4,7-Cl ₄ -DD	-49.0	69.9	606.5	1.703	-6.443	8.670	75.59
2,8-Br ₂ -1,3,6,7-Cl ₄ -DD	-50.7	68.3	606.0	1.703	-6.444	8.670	75.56
2,8-Br ₂ -1,3,7,9-Cl ₄ -DD	-50.9	68.2	605.6	1.705	-6.450	8.675	75.55
2,8-Br ₂ -3,4,6,7-Cl ₄ -DD	-48.0	71.0	605.9	1.702	-6.442	8.670	75.48
1,2-Br ₂ -3,4,6,7,8-Cl ₅ -DD	-55.5	68.8	634.7	1.713	-6.439	8.549	94.74
1,2-Br ₂ -3,6,7,8,9-Cl ₅ -DD	-55.3	68.8	635.6	1.711	-6.433	8.543	94.92
1,3-Br ₂ -2,4,7,8,9-Cl ₅ -DD	-54.7	69.2	636.0	1.712	-6.438	8.547	94.85
1,3-Br ₂ -2,6,7,8,9-Cl ₅ -DD	-53.0	71.0	635.8	1.709	-6.428	8.539	94.99
1,4-Br ₂ -2,3,6,7,8-Cl ₅ -DD	-55.1	68.8	636.2	1.714	-6.445	8.557	94.33
1,6-Br ₂ -2,3,4,7,8-Cl ₅ -DD	-55.0	69.0	635.6	1.714	-6.443	8.554	94.51
1,7-Br ₂ -2,3,4,6,8-Cl ₅ -DD	-54.3	69.9	634.8	1.713	-6.439	8.549	94.74
1,7-Br ₂ -2,3,6,8,9-Cl ₅ -DD	-54.5	69.6	635.3	1.712	-6.436	8.546	94.86
1,8-Br ₂ -2,3,4,7,9-Cl ₅ -DD	-54.6	69.4	635.8	1.712	-6.438	8.548	94.76
1,8-Br ₂ -2,3,6,7,9-Cl ₅ -DD	-54.5	69.4	636.0	1.712	-6.436	8.545	94.93
1,9-Br ₂ -2,3,4,7,8-Cl ₅ -DD	-55.3	68.6	635.9	1.713	-6.441	8.553	94.48
2,3-Br ₂ -1,6,7,8,9-Cl ₅ -DD	-53.3	71.3	633.7	1.709	-6.427	8.538	94.96
2,7-Br ₂ -1,3,4,6,8-Cl ₅ -DD	-53.9	70.6	634.3	1.711	-6.433	8.543	95.01
2,8-Br ₂ -1,3,4,7,9-Cl ₅ -DD	-53.8	70.3	635.3	1.711	-6.433	8.541	95.16

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Compound	$\Delta_f H^\circ$ (298 K)	$\Delta_f G^\circ$ (298 K)	S° (298 K)	$C_p, \text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$			
	$\text{kJ}\cdot\text{mol}^{-1}$	$\text{kJ}\cdot\text{mol}^{-1}$	$\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$	$C_p = A T^3 + B T^2 + C T + D$			
				$A \times 10^7$	$B \times 10^4$	$C \times 10$	D
1,4-Br ₂ -2,3,6,7,8,9-Cl ₆ -DD	-57.0	72.1	665.4	1.720	-6.427	8.422	113.9
1,7-Br ₂ -2,3,4,6,8,9-Cl ₆ -DD	-56.5	73.1	663.9	1.719	-6.424	8.418	114.1
2,3-Br ₂ -1,4,6,7,8,9-Cl ₆ -DD	-56.7	72.8	664.0	1.716	-6.414	8.406	114.7
2,8-Br ₂ -1,3,4,6,7,9-Cl ₆ -DD	-55.9	73.8	663.2	1.718	-6.419	8.411	114.5
1,2,3-Br ₃ -4-Cl ₁ -DD	40.9	135.8	557.9	1.672	-6.424	8.897	37.28
1,2,6-Br ₃ -7-Cl ₁ -DD	25.2	119.2	560.8	1.672	-6.421	8.890	37.56
1,3,7-Br ₃ -2-Cl ₁ -DD	25.1	118.9	561.4	1.671	-6.414	8.874	38.62
1,4,6-Br ₃ -9-Cl ₁ -DD	26.0	118.7	565.4	1.659	-6.385	8.862	37.75
2,3,7-Br ₃ -8-Cl ₁ -DD	14.5	108.5	561.0	1.672	-6.415	8.871	39.03
1,2,3-Br ₃ -7,8-Cl ₂ -DD	4.7	104.6	588.0	1.683	-6.413	8.750	58.23
1,2,4-Br ₃ -6,9-Cl ₂ -DD	10.0	108.7	591.8	1.669	-6.374	8.725	57.96
1,3,7-Br ₃ -2,4-Cl ₂ -DD	19.6	119.2	588.6	1.680	-6.406	8.750	57.88
1,3,7-Br ₃ -2,8-Cl ₂ -DD	8.3	107.9	588.8	1.682	-6.410	8.747	58.37
2,3,7-Br ₃ -8,9-Cl ₂ -DD	9.4	108.7	589.7	1.679	-6.401	8.739	58.53
2,3,8-Br ₃ -1,7-Cl ₂ -DD	7.8	107.2	589.1	1.681	-6.407	8.743	58.57
1,2,3-Br ₃ -6,7,8-Cl ₃ -DD	-0.1	105.1	616.5	1.690	-6.398	8.618	77.80
1,2,4-Br ₃ -6,7,9-Cl ₃ -DD	-2.6	100.6	623.4	1.676	-6.360	8.588	77.97
1,2,6-Br ₃ -4,8,9-Cl ₃ -DD	-2.6	101.0	622.1	1.678	-6.364	8.592	77.87
1,3,7-Br ₃ -2,4,8-Cl ₃ -DD	3.3	108.8	615.7	1.692	-6.405	8.627	77.45
1,3,7-Br ₃ -2,6,8-Cl ₃ -DD	2.0	106.8	617.9	1.693	-6.409	8.628	77.52
2,3,7-Br ₃ -1,6,8-Cl ₃ -DD	1.3	105.9	618.7	1.689	-6.396	8.613	78.11
1,2,3-Br ₃ -4,6,7,8-Cl ₄ -DD	-3.6	106.9	645.3	1.699	-6.392	8.493	97.20
1,2,4-Br ₃ -3,7,8,9-Cl ₄ -DD	-3.3	107.3	644.9	1.701	-6.399	8.502	96.74
1,2,7-Br ₃ -3,4,6,8-Cl ₄ -DD	-2.6	107.8	645.8	1.700	-6.396	8.498	97.00
1,3,7-Br ₃ -2,4,6,8-Cl ₄ -DD	-1.5	109.1	644.8	1.700	-6.396	8.498	97.03
1,3,8-Br ₃ -2,4,7,9-Cl ₄ -DD	-2.0	108.3	646.2	1.700	-6.394	8.495	97.12
2,3,7-Br ₃ -1,4,6,8-Cl ₄ -DD	-2.1	108.5	645.1	1.698	-6.389	8.488	97.49
1,2,3-Br ₃ -4,6,7,8,9-Cl ₅ -DD	-5.6	109.7	675.8	1.704	-6.373	8.359	116.7
1,2,4-Br ₃ -3,6,7,8,9-Cl ₅ -DD	-5.3	110.6	673.7	1.706	-6.381	8.369	116.2
1,2,6-Br ₃ -3,4,7,8,9-Cl ₅ -DD	-5.3	110.2	675.3	1.708	-6.386	8.374	116.0
1,2,7-Br ₃ -3,4,6,8,9-Cl ₅ -DD	-4.7	111.0	674.4	1.706	-6.380	8.365	116.5
1,3,7-Br ₃ -2,4,6,8,9-Cl ₅ -DD	-3.8	111.7	675.5	1.706	-6.378	8.364	116.5
2,3,7-Br ₃ -1,4,6,8,9-Cl ₅ -DD	-4.1	111.0	676.5	1.704	-6.372	8.354	117.0
1,2,3,4-Br ₄ -7-Cl ₁ -DD	65.5	152.2	596.3	1.671	-6.375	8.711	59.75
1,2,3,7-Br ₄ -8-Cl ₁ -DD	59.4	145.6	598.2	1.669	-6.366	8.696	60.52
1,3,7,8-Br ₄ -2-Cl ₁ -DD	61.9	147.8	598.9	1.668	-6.362	8.693	60.50
1,4,6,9-Br ₄ -2-Cl ₁ -DD	65.0	148.8	605.9	1.657	-6.338	8.689	59.21
2,3,7,8-Br ₄ -1-Cl ₁ -DD	61.6	147.6	598.7	1.667	-6.359	8.689	60.73
1,2,3,4-Br ₄ -7,8-Cl ₂ -DD	51.1	142.7	626.5	1.680	-6.364	8.576	79.74
1,2,4,7-Br ₄ -3,8-Cl ₂ -DD	54.8	146.0	627.7	1.680	-6.366	8.579	79.59
1,2,6,7-Br ₄ -3,8-Cl ₂ -DD	51.2	143.0	625.8	1.681	-6.367	8.579	79.59
1,3,7,9-Br ₄ -2,8-Cl ₂ -DD	56.4	147.9	627.1	1.678	-6.357	8.570	79.80
1,4,6,9-Br ₄ -2,7-Cl ₂ -DD	50.0	139.8	632.3	1.668	-6.334	8.559	79.13
2,3,7,8-Br ₄ -1,6-Cl ₂ -DD	54.9	146.2	627.4	1.675	-6.348	8.559	80.29
1,2,3,4-Br ₄ -6,7,8-Cl ₃ -DD	47.6	144.3	656.0	1.686	-6.349	8.443	99.31
1,2,4,8-Br ₄ -3,7,9-Cl ₃ -DD	49.5	146.2	656.0	1.689	-6.355	8.450	99.06
1,2,6,7-Br ₄ -3,4,8-Cl ₃ -DD	48.8	145.9	654.7	1.689	-6.356	8.451	98.96
1,3,6,8-Br ₄ -2,4,7-Cl ₃ -DD	52.1	148.6	656.5	1.687	-6.350	8.445	99.24
1,4,6,9-Br ₄ -2,3,7-Cl ₃ -DD	48.3	143.6	660.6	1.683	-6.343	8.448	98.28
2,3,7,8-Br ₄ -1,4,6-Cl ₃ -DD	51.4	148.4	655.1	1.684	-6.345	8.441	99.46
1,2,3,4-Br ₄ -6,7,8,9-Cl ₄ -DD	45.4	147.4	685.1	1.692	-6.331	8.310	118.8
1,2,4,7-Br ₄ -3,6,8,9-Cl ₄ -DD	47.5	148.6	687.9	1.694	-6.338	8.317	118.6
1,2,6,7-Br ₄ -3,4,8,9-Cl ₄ -DD	46.3	148.6	684.1	1.696	-6.345	8.324	118.2
1,3,6,8-Br ₄ -2,4,7,9-Cl ₄ -DD	48.5	150.4	685.0	1.696	-6.343	8.322	118.4
1,4,6,9-Br ₄ -2,3,7,8-Cl ₄ -DD	46.7	148.2	686.3	1.698	-6.353	8.336	117.6

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Compound	$\Delta_f H^\circ$ (298 K)	$\Delta_f G^\circ$ (298 K)	S° (298 K)	$C_p, \text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$			
	$\text{kJ}\cdot\text{mol}^{-1}$	$\text{kJ}\cdot\text{mol}^{-1}$	$\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$	$C_p = A T^3 + B T^2 + C T + D$			
				$A \times 10^7$	$B \times 10^4$	$C \times 10$	D
2,3,7,8-Br ₄ -1,4,6,9-Cl ₄ -DD	47.9	150.0	684.6	1.692	−6.328	8.302	119.4
1,2,3,4,7-Br ₅ -8-Cl ₁ -DD	105.8	183.4	637.7	1.665	−6.315	8.519	82.14
1,2,3,6,7-Br ₅ -8-Cl ₁ -DD	104.6	181.9	638.9	1.665	−6.312	8.517	82.15
1,2,3,7,8-Br ₅ -6-Cl ₁ -DD	106.5	184.2	637.3	1.663	−6.306	8.510	82.40
1,2,4,6,9-Br ₅ -7-Cl ₁ -DD	103.2	178.2	646.3	1.653	−6.282	8.502	81.42
1,2,4,7,8-Br ₅ -3-Cl ₁ -DD	108.6	186.0	638.2	1.665	−6.315	8.522	81.86
1,2,3,4,6-Br ₅ -7,8-Cl ₂ -DD	99.6	182.5	666.9	1.675	−6.309	8.396	101.3
1,2,3,6,7-Br ₅ -4,8-Cl ₂ -DD	100.6	184.0	665.0	1.675	−6.308	8.395	101.4
1,2,3,7,8-Br ₅ -6,9-Cl ₂ -DD	102.4	185.8	664.8	1.671	−6.297	8.383	101.8
1,2,4,6,8-Br ₅ -3,7-Cl ₂ -DD	103.1	186.0	666.6	1.675	−6.309	8.398	101.1
1,2,4,6,9-Br ₅ -3,7-Cl ₂ -DD	100.1	181.9	670.4	1.669	−6.295	8.390	101.0
1,2,4,7,9-Br ₅ -3,8-Cl ₂ -DD	102.9	185.6	667.4	1.674	−6.308	8.397	101.2
1,2,3,4,6-Br ₅ -7,8,9-Cl ₃ -DD	97.3	185.6	695.1	1.682	−6.296	8.268	120.6
1,2,3,7,8-Br ₅ -4,6,9-Cl ₃ -DD	99.1	187.7	694.1	1.680	−6.289	8.257	121.3
1,2,3,8,9-Br ₅ -4,6,7-Cl ₃ -DD	97.9	185.9	696.2	1.681	−6.294	8.264	120.9
1,2,4,6,8-Br ₅ -3,7,9-Cl ₃ -DD	99.2	186.8	697.2	1.683	−6.301	8.273	120.4
1,2,4,6,9-Br ₅ -3,7,8-Cl ₃ -DD	98.3	185.7	698.2	1.685	−6.307	8.283	119.9
1,2,4,8,9-Br ₅ -3,6,7-Cl ₃ -DD	98.4	186.3	696.4	1.683	−6.301	8.273	120.5
1,2,3,4,6,7-Br ₆ -8-Cl ₁ -DD	151.5	220.7	676.7	1.661	−6.263	8.343	103.6
1,2,3,4,6,9-Br ₆ -7-Cl ₁ -DD	151.1	219.3	680.2	1.655	−6.244	8.330	103.5
1,2,3,4,7,8-Br ₆ -6-Cl ₁ -DD	153.8	222.5	678.7	1.659	−6.256	8.335	103.9
1,2,3,6,7,8-Br ₆ -4-Cl ₁ -DD	154.1	223.7	675.4	1.660	−6.257	8.337	103.8
1,2,4,6,8,9-Br ₆ -3-Cl ₁ -DD	153.2	221.1	681.1	1.654	−6.243	8.332	103.2
1,2,3,4,6,7-Br ₆ -8,9-Cl ₂ -DD	149.2	224.0	704.7	1.669	−6.252	8.216	122.9
1,2,3,4,6,9-Br ₆ -7,8-Cl ₂ -DD	149.2	223.2	707.3	1.670	−6.257	8.223	122.5
1,2,3,4,7,8-Br ₆ -6,9-Cl ₂ -DD	150.0	223.6	708.7	1.667	−6.245	8.206	123.5
1,2,3,6,7,8-Br ₆ -4,9-Cl ₂ -DD	150.1	224.8	705.0	1.668	−6.249	8.210	123.3
1,2,4,6,7,9-Br ₆ -3,8-Cl ₂ -DD	149.9	224.2	706.4	1.671	−6.261	8.227	122.3
1,2,3,4,6,7,8-Br ₇ -9-Cl ₁ -DD	201.1	262.1	715.4	1.655	−6.204	8.159	125.4
1,2,3,4,6,7,9-Br ₇ -8-Cl ₁ -DD	200.8	259.8	721.8	1.656	−6.209	8.167	124.9

^aV. P. Kolesov, O. V. Dorofeeva, V. S. Iorish, T. S. Papina, V. A. Luckyanova and S. V. Melkhanova: Organohalogen Compounds 36 (1998), 201-204.