*Thermochimica Acta*, 112 (1987) 117–122
Elsevier Science Publishers B.V., Amsterdam – Printed in The Netherlands

# PREDICTION OF VAPOR PRESSURES, BOILING POINTS AND ENTHALPIES OF FUSION FOR TWENTY-NINE HALOGENATED DIBENZO-P-DIOXINS

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## ABSTRACT

A vapor pressure correlation method was used to predict vapor pressures for 15 polychloro-, 8 polybromo-, 2-iodo-, 2,3-difluoro- and 4 mixed halogenated dibenzo-p-dioxins. Experimental vapor pressures, obtained on 10 chlorinated dibenzo-p-dioxins, were used as data base for the predictions. The correlation method uses the liquids as reference states. Boiling points and enthalpies of fusion were deduced for the measured compounds and were correlated with the degree of halogenation. The calculated boiling points and enthalpies of fusion are in good agreement with observed values. The two correlations were used to predict boiling points and enthalpies of fusion for related dioxins of known melting points, and these values served as starting point for the vapor pressure predictions. Molar heat capacities of the gaseous and the liquid phases, enthalpies and entropies of evaporation, of sublimation and of fusion were also estimated for the investigated halogenated dibenzo-p-dioxins.

## INTRODUCTION

Modeling of the environmental fate of hazardous compounds and of their behaviour in industrial processes (i.e. incineration) is only possible if some basic physico chemical substance properties are known. Some properties such as binary diffusion rates and heat capacities in the liquid or gaseous phase can be estimated with sufficient accuracy for modeling purposes (refs. 1-2). Other parameters like melting points, enthalpies of fusion and vapor pressures must be measured. Using correlation methods, these properties can alternatively be deduced from experimental data of related compounds (refs. 3-5).

Correlation methods are of particular importance when dealing with halogenated dibenzo-p-dioxins and dibenzo-furans since there are hundreds of homologues and isomers (e.g. 75 dioxins and 135 furans for chlorine substitution alone). The synthesis of pure compounds can be very difficult. Acordingly most species have only been identified by GC-MS techniques in mixtures and have been synthesized at trace levels (refs. 6-8). Many of the compounds are highly toxic and their impact on the environment must be considered along with the hazards of 2,3,7,8-TCDD. The measurement of thermodynamic properties generally requires milligram quantities and safe experimentation can be very involved. Correlation methods permit estimates of substance properties for hundreds of compounds from a limited set of measurements on the least toxic species.

Correlation methods allow testing of the experimental data set for self consistency. Calculation of related substance properties should become possible (i.e. boiling points and enthalpies of fusion from vapor pressure data). The method used can then be tested by a comparison of predicted and observed values.

0040-6031/87/$03.50

## VAPOR PRESSURE CORRELATION METHOD

The correlation method is based on entropies of evaporation at the boiling point ($T_b$) since they are relatively independent of substance and therefore reliably predictable (ref. 3). Fishtine's formula, $s_v(T_b) = 1.01\ (36.61 + R \ln T_b) + R \ln P^o$ ($P^o = 1.01325$ Pa), was used to predict the entropies of evaporation for the different compounds at $T_b$. The enthalpies of evaporation at $T_b$ are similarly obtained by $h_v = 1.01\ T_b\ (36.61 + R \ln T_b)$. The boiling points $T_b$ can be calculated by iteration for the set of polychlorinated dibenzo-p-dioxins whose sublimation pressures have been measured.

Figure 1 illustrates the procedure. The sublimation pressures are extrapolated to the melting points ($T_m$) were they equal the vapor pressures of the liquids. The latter can be calculated (refs. 3, 5) for given boiling points: $\ln P(T_m) = \ln P^o - (h_v(T_b) / R\ T_b)\ \{(1+K)(T_b/T_m - 1) - K \ln (T_b/T_m)\}$ with $K = -T_b\ c_p^{gas-liquid} / h_v(T_b)$. This entails extrapolations along the strongly bent vapor pressure curves of the liquid compounds (Fig. 1).

The temperature dependencies of the enthalpies of sublimation and evaporation are given by $h_v(T_1) = h_v(T_2) + (T_1 - T_2)\ c_p^{gas\ -\ solid\ (or\ liquid)}$. A fixed value of $c_p^{gas\ -\ solid} = -2R$ ($R = 8.3143$ J/mol K) was assumed using the rule of Dulong and Petit for the solid. The heat capacity changes between the liquids and the gases are much smaller and the heat capacities were estimated by the group contribution methods by Chue and Swanson for the liquids at 20°C and by Benson and Cruickshank for the gases.

The enthalpies and entropies of evaporation can now be calculated for $T_m$ ; $h_v(T_m) = h_v(T_b)\ \{1 + K\ (1 - T_m/T_b)\}$ and $s_v(T_m) = R \ln P_{liquid}(P_m) + h_v(T_m)/T_m$. Similarly the enthalpies and entropies of fusion can be obtained for the melting points by $h_m(T_m) = h_s(T_m) - h_v(T_m)$ and $s_m(T_m) = h_m(T_m) / T_m$. Finally the entropy of sublimation $s_s(T_m)$ can be determined by $s_m(T_m) = s_s(T_m) - s_v(T_m)$.

Vapor pressures were measured for a number of solid polychloro dibenzo-p-dioxins, dibenzofurans and related compounds (refs. 3, 9-11). Table 1 and the upper part of Table 2 shows the different parameters that were obtained from this set of experimental enthalpies and entropies of sublimation (note: Table 1 rectifies faulty $c_p$ values (ref.3) for xanthene, 1,2,4,5,7,8-hexachloroxanthene and 9,10-dihydroanthracene). The calculated boiling points and enthalpies of fusion compare nicely with the few available experimental values (Fig. 2).

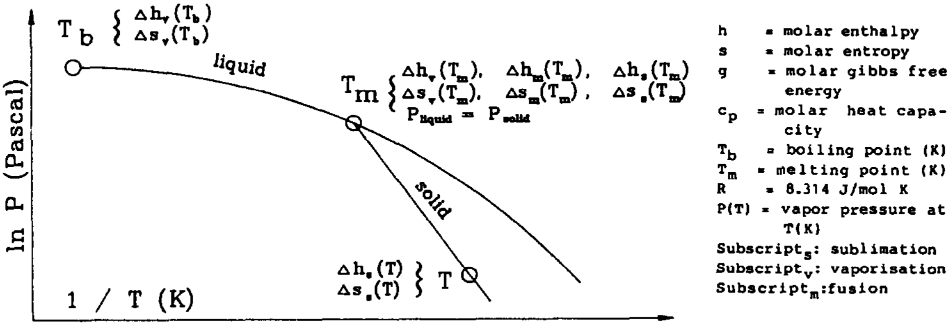

Fig. 1. Diagram showing the temperature dependence of vapor pressures.

TABLE 1 Observed (obs.), extrapolated (extr.), estimated (est.) and predicted (pred.) values of parameters used in the vapor pressure correlation method for dibenzofuran (DF), three polychlorodibenzofurans and related compounds.

| | hs (J/mol) | ss (J/mol K) | meas.range ( C) | tm ( C) | lnP(Tm) (Pa) | cp(g-l) (J/mol K) | K | sv(Tb) | sv(Tm) | hv(Tm) (kJ/ mol) | sm(Tm) (J/ mol K) | hm(Tm) (kJ/mol) | | Tb ( C) | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | obs. | obs. | obs. | obs. | extr. | est. | | (J/mol K) | | | | pred. | obs. | pred. | obs. |
| DF | 85630 | 278.49 | 31 - 70 | 86.5 | 4.85 | -87.6 | 0.97 | 185.7 | 224 | 65.4 | 54 | 19.6 | | 273 | 287 |
| 36-DCDF | 110870 | 300.9 | 32 - 101 | 188 | 7.03 | -78.7 | 0.86 | 186.9 | 226 | 70.7 | 75 | 34.5 | 32.4 | 357 | |
| 248-TCDF | 112300 | 299.31 | 45 - 150 | 154 | 4.35 | -74.3 | 0.81 | 187.4 | 223 | 78.7 | 76 | 32.6 | | 392.5 | (375) |
| OCDF | 149430 | 323.07 | 100 - 201 | 259 | 5.03 | -52.1 | 0.56 | 189.0 | 215 | 90.0 | 108 | 57.5 | | 537 | |
| Xanthene | 92450 | 284.79 | 32 - 80 | 100.5 | 4.48 | -96.0 | 1.06 | 186.1 | 229 | 71.0 | 55 | 20.7 | | 300.5 | 311 |
| 124578-HCX | 147000 | 331.32 | 80 - 176 | 261.5 | 6.70 | -69.4 | 0.75 | 188.3 | 216 | 83.2 | 115 | 61.5 | | 470 | |
| Anthracene | 98745 | 274.38 | 45 - 100 | 215.8 | 8.50 | -79.0 | 0.87 | 186.7 | 216 | 65.5 | 59 | 28.6 | 29.4 | 340 | 340 |
| DH-Anthr. | 93221 | 284.96 | 31 - 96 | 111 | 5.07 | -78.7 | 0.87 | 186.2 | 221 | 67.8 | 64 | 24.6 | | 306.5 | 305 |

PREDICTION OF VAPOR PRESSURES FOR HALOGENATED DIBENZO-P-DIOXINS

The connection between the measured polychloro dibenzo-p-dioxins and the related halogenated compounds of unknown vapor pressures is established by correlations of the calculated enthalpies of fusion and boiling points with the degree of chlorine substitution (X) (ref. 3): $h_m(T_m) = 13.61 + 5.75\ X \pm 2$ kJ/mol and $T_b = 283 + 42.0\ X - 1.73\ X^2 \pm 15$ K. To my knowledge vapor pressures have so far only been measured for chlorinated dioxins and the validity of the two correlation equations for other halogenated species presently cannot be verified. The investigated polychlorodibenzofurans and xanthens followed the same dependencies however and this suggests that the equations can be extended to other halogen substitution (ref. 3).

After estimating the boiling points for the unknown dioxins, one can calculate the entropies and the enthalpies of evaporation at $T_b$ by the Fishtine formula. The heat capacities of the gases and the liquids are then estimated. The estimates permit one to obtain the temperature dependencies of the vapor pressures, the enthalpies and entropies of evaporation and allow evaluation of the parameters for the melting point. The enthalpies and entropies of sublimation at $T_m$ are then calculated and the enthalpies of fusion are derived from the correlation. These values are recalculated for $T_{mid}(K) = Tmin\ T_{max} / (T_{min} + T_{max})$ for the range between 25 and 100°C (Table 2, predicted values of $h_s$ and $s_s$) by using the temperature dependencies of the enthalpies and entropies of sublimation, $h_s(T_1) = h_s(T_2) + c_p^{gas\ -\ solid}(T_1 - T_2)$ and $s_s(T_1) = s_s(T_2) + c_p^{gas\ -\ solid}\ln(T_1/T_2)$. The vapor pressures shown in Table 2 were calculated using these values in the linear relation, $RT\ln P(Pa) = T\ s_s(T_{mid}) - h_s(_{mid})$.

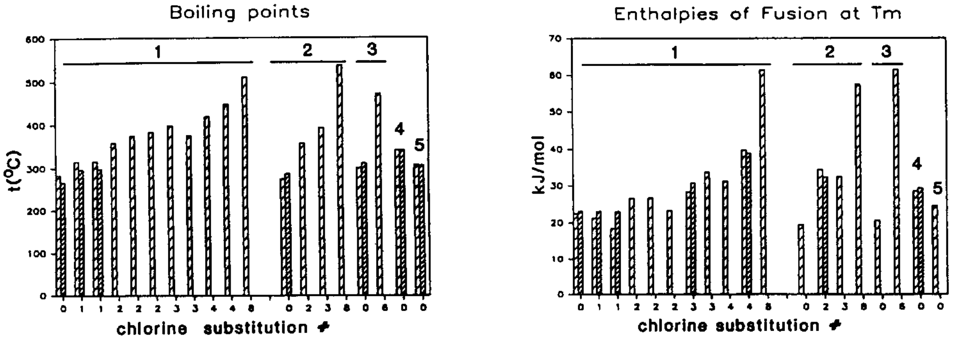

Fig.2 Comparison of calculated ▭ and observed ▨ values for dibenzo-p-dioxins (1), dibenzofurans (2), xanthens (3), anthracene (4) and dihydroanthracene (5).

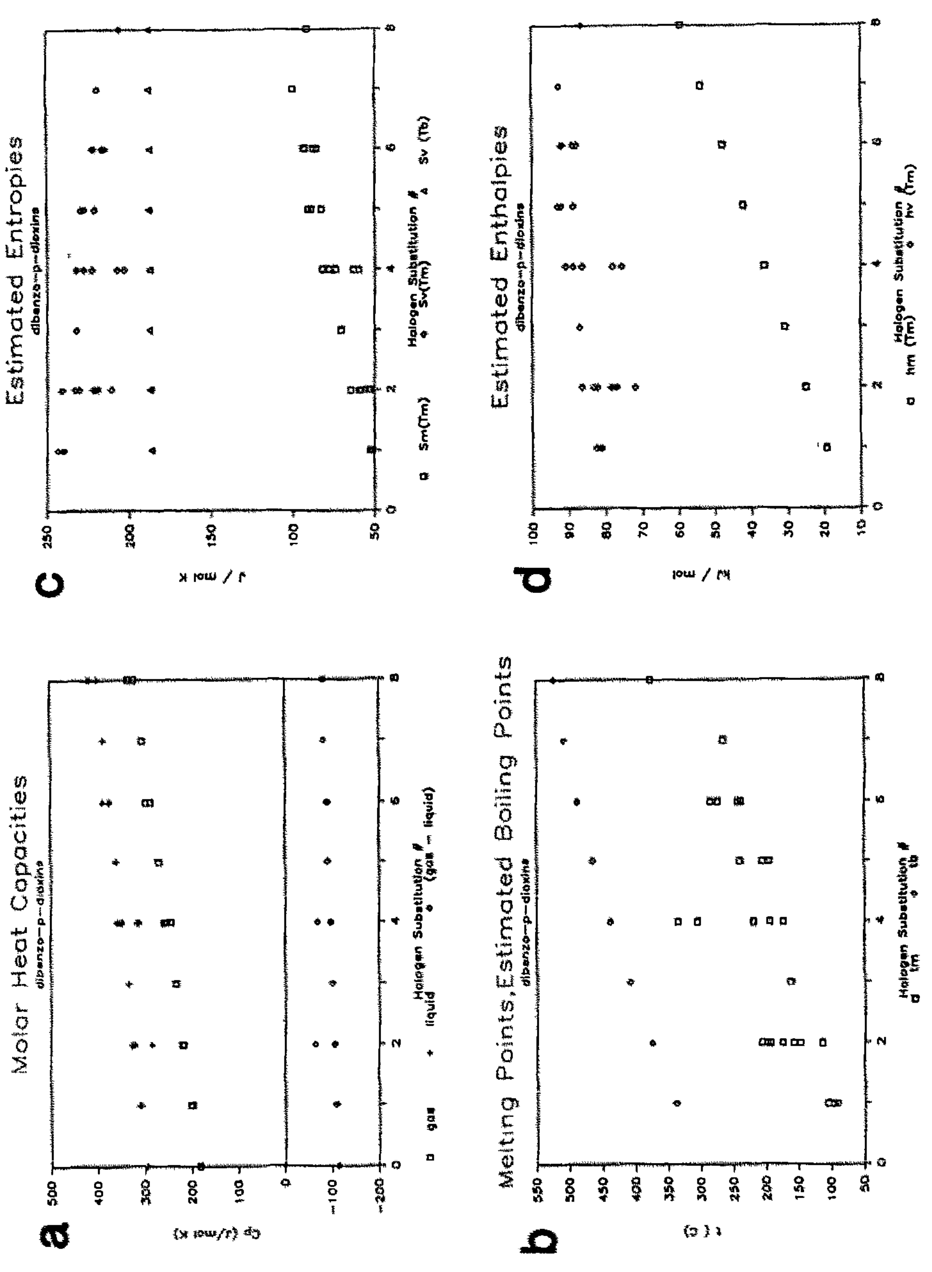

Fig. 3 Halogen correlations of thermal properties of halogenated dibenzo-p-dioxins. The plots include only entries for the compounds of unknown vapor pressures (Table 2, bottom part). a) Molar heat capacities estimated by group contribution methods for the gases and the liquids. b) Experimental melting points and predicted boiling points from the chlorine correlation of calculated boiling points (ref. 3). c) Entropies of evaporation at $T_m$ and $T_b$ and entropies of fusion at $T_m$ (from top to bottom). d) Enthalpies of evaporation and of fusion at $T_m$ (from top to bottom).

TABLE 2

Vapor pressure correlation (top) and vapor pressure predictions (bottom) for polyhalogenated dibenzo-p-dioxins. Shown is the LOTUS 1-2-3 spreadsheet which includes from left to right: enthalpies and entropies of sublimation, melting point range - literature values, heat capacity change from liquid to gas, constant K (see text), entropies of evaporation at $T_b$ and $T_m$, enthalpies of evaporation at $T_m$, entropies and enthalpies of fusion at $T_m$ and boiling points. The vapor pressures of the solids have been calculated for various temperatures using the enthalpies and entropies of sublimation shown for $t_{mid}$ = 62.3°C.

| | hs (J/mol) obs. | ss (J/mol K) obs. | melting point tm ( C) obs. | | lit. | cp(g-l) (J/mol K) est. | K | sv(Tb) (J/mol K) | sv(Tm) (J/mol K) | hv(Tm) (kJ/mol) | sm(Tm) (J/mol K) | hm(Tm) (kJ/mol) pred. | Tb ( C) pred. | vapor pressures for t( C) 25 P(Pa) experimental (inter-, extrapolations) | 50 | 75 | 100 | 125 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| DD | 92250 | 285.29 | 122 | 123 | 1 | -113.3 | 1.26 | 185.9 | 228 | 68.4 | 57 | 22.6 | 283.5 | 5.5E-02 | 9.8E-01 | 1.2E+01 | 9.7E+01 | 6.3E+02 |
| 1-MCDD | 98550 | 293.8 | 104.5 | 105.5 | 1 | -108.9 | 1.20 | 186.4 | 237 | 76.2 | 56 | 21.4 | 315.5 | 1.2E-02 | 2.6E-01 | 3.6E+00 | 3.6E+01 | 2.6E+02 |
| 2-MCDD | 97160 | 292.1 | 88 | 89 | 1 | -108.9 | 1.20 | 186.4 | 241 | 78.1 | 51 | 18.5 | 316 | 1.7E-02 | 3.6E-01 | 4.8E+00 | 4.5E+01 | 3.2E+02 |
| 23-DCDD | 106230 | 291.08 | 163 | 164 | 1 | -104.5 | 1.15 | 186.9 | 230 | 77.8 | 61 | 26.7 | 358 | 3.9E-04 | 1.1E-02 | 1.8E-01 | 2.2E+00 | 1.9E+01 |
| 27-DCDD | 105510 | 279.05 | 209 | 210 | 1 | -104.5 | 1.14 | 187.2 | 224 | 76.4 | 55 | 26.8 | 374.5 | 1.2E-04 | 3.3E-03 | 5.6E-02 | 6.4E-01 | 5.4E+00 |
| 28-DCDD | 109010 | 291.87 | 150.5 | 151 | 1 | -104.5 | 1.14 | 187.3 | 237 | 84.1 | 55 | 23.3 | 382.5 | 1.4E-04 | 4.2E-03 | 7.8E-02 | 9.7E-01 | 8.8E+00 |
| 137-T3CDD | 116200 | 304.77 | 148.5 | 148.6 | 10 | -100.0 | 1.09 | 187.5 | 237 | 86.4 | 67 | 28.4 | 398 | 3.6E-05 | 1.4E-03 | 3.1E-02 | 4.5E-01 | 4.7E+00 |
| 124-T3CDD | 118790 | 322.16 | 128 | 129 | 1 | -100.0 | 1.09 | 187.2 | 238 | 83.9 | 84 | 33.9 | 375 | 1.0E-04 | 4.2E-03 | 1.0E-01 | 1.6E+00 | 1.8E+01 |
| 1234-T4CDD | 118530 | 298.15 | 188 | 190 | 2 | -95.6 | 1.04 | 187.7 | 231 | 85.6 | 68 | 31.2 | 419 | 6.4E-06 | 2.6E-04 | 6.2E-03 | 9.6E-02 | 1.1E+00 |
| 2378-T4CDD | 124001 | 287.6 | 305 | 306 | 1 | -95.6 | 1.04 | 188.1 | 219 | 79.9 | 69 | 39.9 | 446.5 | 2.0E-07 | 9.5E-06 | 2.6E-04 | 4.6E-03 | 5.7E-02 |
| OCDD | 151130 | 316.48 | 330 | 332 | 1 | -77.9 | 0.84 | 188.8 | 215 | 86.7 | 102 | 61.4 | 510 | 1.1E-10 | 1.3E-08 | 7.2E-07 | 2.4E-05 | 5.1E-04 |
| | pred. | pred. | | | | | | | | | | | | P(Pa) predicted | | | | |
| 13-DCDD | 112542 | 309 | 113.5 | 114.5 | 2 | -104.5 | 1.14 | 187.2 | 241 | 86.5 | 65 | 25.1 | 375.0 | 2.5E-04 | 8.4E-03 | 1.7E-01 | 2.3E+00 | 2.2E+01 |
| 16-DCDD | 105156 | 280 | 197 | 199 | 3 | -104.5 | 1.14 | 187.2 | 221 | 77.7 | 53 | 25.1 | 375.0 | 1.5E-04 | 4.1E-03 | 6.8E-02 | 7.7E-01 | 6.5E+00 |
| 237-T3CDD | 119759 | 308 | 162 | 163 | 4 | -100.0 | 1.09 | 187.6 | 232 | 87.2 | 71 | 30.9 | 408.4 | 1.2E-05 | 5.2E-04 | 1.3E-02 | 2.1E-01 | 2.3E+00 |
| 2378-T4CDD | 118976 | 280 | 305 | 306 | 1 | -95.64 | 1.04 | 188.0 | 208 | 78.2 | 63 | 36.6 | 438.3 | 6.2E-07 | 2.6E-05 | 6.1E-04 | 9.7E-03 | 1.1E-01 |
| 1237-T4CDD | 129410 | 319 | 172 | 175 | 11 | -95.64 | 1.04 | 188.0 | 232 | 90.9 | 82 | 36.6 | 438.3 | 1.0E-06 | 5.9E-05 | 1.9E-03 | 3.7E-02 | 5.1E-01 |
| 1368-T4CDD | 125794 | 304 | 219 | 219.5 | 1 | -95.64 | 1.04 | 188.0 | 223 | 86.5 | 74 | 36.6 | 438.3 | 7.0E-07 | 3.6E-05 | 1.0E-03 | 1.9E-02 | 2.4E-01 |
| 1378-T4CDD | 127770 | 312 | 193.5 | 195 | 2 | -95.64 | 1.04 | 188.0 | 228 | 88.9 | 78 | 36.6 | 438.3 | 8.4E-07 | 4.5E-05 | 1.4E-03 | 2.6E-02 | 3.5E-01 |
| 12347-PCDD | 137419 | 326 | 195 | 196 | 1 | -91.21 | 0.99 | 188.3 | 230 | 92.8 | 90 | 42.4 | 464.7 | 8.8E-08 | 6.4E-06 | 2.5E-04 | 6.1E-03 | 9.8E-02 |
| 12378-PCDD | 134062 | 311 | 240 | 241 | 4 | -91.21 | 0.99 | 188.3 | 221 | 88.7 | 83 | 42.4 | 464.7 | 5.8E-08 | 3.8E-06 | 1.4E-04 | 3.0E-03 | 4.6E-02 |
| 12478-PCDD | 136636 | 322 | 206 | 206 | 4 | -91.21 | 0.99 | 188.3 | 228 | 91.8 | 88 | 42.4 | 464.7 | 7.8E-08 | 5.6E-06 | 2.1E-04 | 5.1E-03 | 8.0E-02 |
| 123478-H6CDD | 140782 | 313 | 273 | 275 | 1 | -86.77 | 0.94 | 188.5 | 217 | 89.1 | 88 | 48.1 | 487.7 | 5.1E-09 | 4.1E-07 | 1.8E-05 | 4.6E-04 | 8.0E-03 |
| 124679-H6CDD | 143238 | 324 | 238 | 240 | 1 | -86.77 | 0.94 | 188.5 | 223 | 92.1 | 94 | 48.1 | 487.7 | 6.8E-09 | 5.9E-07 | 2.7E-05 | 7.5E-04 | 1.4E-02 |
| 123678-H6CDD | 139975 | 310 | 285 | 286 | 6 | -86.77 | 0.94 | 188.5 | 215 | 88.1 | 86 | 48.1 | 487.7 | 4.8E-09 | 3.8E-07 | 1.6E-05 | 4.0E-04 | 6.9E-03 |
| 123789-H6CDD | 142922 | 323 | 243 | 244 | 6 | -86.77 | 0.94 | 188.5 | 222 | 91.7 | 93 | 48.1 | 487.7 | 6.5E-09 | 5.6E-07 | 2.6E-05 | 7.0E-04 | 1.3E-02 |
| 1234678-H7CDD | 149792 | 328 | 264 | 265 | 11 | -82.34 | 0.89 | 188.7 | 219 | 92.5 | 100 | 53.9 | 507.2 | 7.5E-10 | 8.0E-08 | 4.4E-06 | 1.4E-04 | 2.9E-03 |
| 1-MBDD | 101300 | 293 | 104 | 106 | 5 | -109.7 | 1.21 | 186.7 | 239 | 81.2 | 51 | 19.4 | 338.2 | 3.5E-03 | 8.4E-02 | 1.3E+00 | 1.3E+01 | 1.0E+02 |
| 2-MBDD | 102604 | 298 | 90 | 92 | 5 | -109.7 | 1.21 | 186.7 | 244 | 82.7 | 53 | 19.4 | 338.2 | 4.0E-03 | 9.9E-02 | 1.5E+00 | 1.7E+01 | 1.3E+02 |
| 23-DBDD | 109059 | 293 | 157.5 | 158 | 2 | -106.1 | 1.16 | 187.2 | 231 | 82.3 | 58 | 25.1 | 375.0 | 1.6E-04 | 4.9E-03 | 9.0E-02 | 1.1E+00 | 1.0E+01 |
| 27-DBDD | 105856 | 282 | 193 | 194 | 7 | -106.1 | 1.16 | 187.2 | 222 | 78.5 | 54 | 25.1 | 375.0 | 1.5E-04 | 4.0E-03 | 6.7E-02 | 7.8E-01 | 6.6E+00 |
| 16-DBDD | 104646 | 278 | 207 | 207 | 7 | -106.1 | 1.16 | 187.2 | 219 | 77.1 | 52 | 25.1 | 375.0 | 1.5E-04 | 3.8E-03 | 6.2E-02 | 7.0E-01 | 5.8E+00 |
| 28-DBDD | 109977 | 297 | 145 | 150 | 5 | -106.1 | 1.16 | 187.2 | 233 | 83.4 | 60 | 25.1 | 375.0 | 1.7E-04 | 5.3E-03 | 1.0E-01 | 1.3E+00 | 1.2E+01 |
| 2378-T4BDD | 116990 | 274 | 334 | 336 | 2 | -98.99 | 1.07 | 188.0 | 203 | 75.8 | 60 | 36.6 | 438.3 | 6.4E-07 | 2.5E-05 | 5.6E-04 | 8.4E-03 | 9.0E-02 |
| OBDD | 151497 | 309 | 376 | 376 | 9 | -84.60 | 0.91 | 188.9 | 206 | 86.6 | 92 | 59.6 | 523.2 | 4.1E-11 | 4.6E-09 | 2.6E-07 | 8.8E-06 | 1.9E-04 |
| 2-MIDD | 101530 | 295 | 95 | 97 | 5 | -107.2 | 1.18 | 186.7 | 241 | 81.5 | 52 | 19.4 | 338.2 | 4.2E-03 | 1.0E-01 | 1.5E+00 | 1.6E+01 | 1.2E+02 |
| 23-DFDD | 99142 | 272 | 174 | 176 | 2 | -64.35 | 0.70 | 187.2 | 211 | 72.1 | 56 | 25.1 | 375.0 | 6.9E-04 | 1.5E-02 | 2.1E-01 | 2.1E+00 | 1.6E+01 |
| 23-DB-78-DCDD | 118290 | 278 | 316 | 317.5 | 2 | -97.32 | 1.06 | 188.0 | 206 | 77.4 | 62 | 36.6 | 438.3 | 6.2E-07 | 2.5E-05 | 5.8E-04 | 9.0E-03 | 9.9E-02 |
| 23-DC-78-DFDD | 119500 | 293 | 223 | 225 | 2 | -68.03 | 0.74 | 188.0 | 212 | 80.1 | 74 | 36.6 | 438.3 | 2.3E-06 | 9.4E-05 | 2.3E-03 | 3.7E-02 | 4.1E-01 |
| 23-DB-78-DFDD | 120549 | 297 | 210 | 212 | 2 | -69.70 | 0.76 | 188.0 | 215 | 81.4 | 76 | 36.6 | 438.3 | 2.4E-06 | 1.0E-04 | 2.6E-03 | 4.2E-02 | 4.8E-01 |
| 124679-H6B-<br>-38-DCDD | 150554 | 306 | 385 | 388 | 8 | -82.92 | 0.89 | 188.9 | 205 | 85.5 | 90 | 59.6 | 523.2 | 4.2E-11 | 4.6E-09 | 2.6E-07 | 8.5E-06 | 1.8E-04 |

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## DISCUSSION

The present method is limited to compounds with known melting points. Table 2 lists all of the halogenated dibenzo-p-dioxins for which this is the case. The close agreement between melting points for common isomers with different halogen substitution (see Fig. 3b) is further indication that the chlorine correlations may be applied to other halogenated dioxins.

1,6-, 2,7- and 2,3,7,8- isomers have high melting points. This is a manifestation of high lattice energies in the solid phases. The relatively high stabilities of the solids are in turn reflected by predictions of low sublimation pressures (Table 2). Such extra stabilization for given isomers enters the model only by way of the melting points. The present model could be refined by including this effect in the predictions of enthalpies of fusion and boiling points (see Fig. 3; $h_m$ and $T_b$ are predicted in this correlation method only as a function of the degree of halogenation).

This fact could explain the observed differences between the present vapor pressure predictions and experimental values for 2,3,7,8-TCDD (ref. 10, 11; the predicted pressures lie higher by a factor of 2 to 4). An overestimation is also expected for the the brominated analog, 2,3,7,8-TBDD. A much closer agreement with observations is expected for the remaining compounds. Predictions are in very good agreement indeed where comparisons with measurements are possible (ref. 13; data at 30 and 40°C extrapolated to 25°C, values in brackets): $10^{-6}$ Pa ($10^{-6}$ Pa) for 1,2,3,4-$T_4$CDD, $9\times10^{-8}$ Pa ($6\times10^{-8}$ Pa) for 1,2,3,4,7-$P_5$CDD, $5\times10^{-9}$ Pa ($3\times10^{-8}$ Pa) for 1,2,3,4,7,8-$H_6$CDD and $7.5\times10^{-10}$ Pa ($5\times10^{-9}$ Pa) for 1,2,3,4,6,7,8-$H_7$CDD. The observed values for the last two compounds are probably somewhat high (ref. 13, tailing of the observed vapor pressure curves).

It has been shown that chlorinated dibenzofurans and xanthens follow the same correlations (ref. 3) and vapor pressure predictions will be possible for these compounds.

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