# 1,2,4-Trichlorodibenzo-p-dioxin

| | |
|---|---|
| **Other names:** | 1,2,4-Trichlorodibenzo-para-dioxin |
| | 1,2,4-Trichlorodibenzo[b,e] [1,4]dioxin |
| | 1,2,4-Trichlorodibenzodioxin |
| | 1,2,4-trichlorooxanthrene |
| | Dibenzo-p-dioxin, 1,2,4-trichloro- |
| **Inchi:** | InChI=1S/C12H5Cl3O2/c13-6-5-7(14)11-12(10(6)15)17-9-4-2-1-3-8(9)16-11/h1-5H |
| **InchiKey:** | HRVUKLBFRPWXPJ-UHFFFAOYSA-N |
| **Formula:** | C12H5Cl3O2 |
| **SMILES:** | Clc1cc(Cl)c2c(c1Cl)Oc1ccccc1O2 |
| **Mol. weight [g/mol]:** | 287.53 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -82.29 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 40.69 | kJ/mol | Joback Method |
| ie | 8.02 | eV | Cheméo Relay (1.0) |
| log10ws | -7.60 | | Aqueous Solubility Prediction Method |
| logp | 5.545 | | Crippen Method |
| mcvol | 170.020 | ml/mol | McGowan Method |
| rinpol | 2152.00 | | NIST Webbook |
| rinpol | 2152.00 | | NIST Webbook |
| rinpol | 2176.00 | | NIST Webbook |
| rinpol | 2176.00 | | NIST Webbook |
| rinpol | 2143.00 | | NIST Webbook |
| rinpol | 2152.00 | | NIST Webbook |
| rinpol | 2143.00 | | NIST Webbook |
| tf | 398.84 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 419.96 | J/mol×K | 990.47 | Joback Method |
| cpg | 406.87 | J/mol×K | 902.16 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 374.96 | J/mol×K | 725.55 | Joback Method |
| cpg | 383.94 | J/mol×K | 769.70 | Joback Method |
| cpg | 392.18 | J/mol×K | 813.86 | Joback Method |
| cpg | 399.78 | J/mol×K | 858.01 | Joback Method |
| cpg | 413.56 | J/mol×K | 946.32 | Joback Method |
| dvisc | 0.0013574 | Pa×s | 509.04 | Joback Method |
| dvisc | 0.0010829 | Pa×s | 545.12 | Joback Method |
| dvisc | 0.0008885 | Pa×s | 581.21 | Joback Method |
| dvisc | 0.0007461 | Pa×s | 617.30 | Joback Method |
| dvisc | 0.0006387 | Pa×s | 653.38 | Joback Method |
| dvisc | 0.0005557 | Pa×s | 689.47 | Joback Method |
| dvisc | 0.0004903 | Pa×s | 725.55 | Joback Method |
| hsubt | 121.00 ± 1.80 | kJ/mol | 365.50 | NIST Webbook |
| hsubt | 118.80 | kJ/mol | 342.00 | NIST Webbook |

# Sources

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Cheméo Relay (1.0):**
**Cheméo Relay (1.0, beta):**
**Aqueous Solubility Prediction Method:** http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C39227582&Units=SI

# Legend

**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**hf:** Enthalpy of formation at standard conditions
**hfus:** Enthalpy of fusion at standard conditions
**hsubt:** Enthalpy of sublimation at a given temperature
**ie:** Ionization energy
**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume
**rinpol:** Non-polar retention indices
**tf:** Normal melting (fusion) point