# Dibenzodioxin, 2,8-dibromo-, 3,7-dichloro-

**Inchi:** InChI=1S/C12H3Br2Cl3O2/c13-4-1-7-8(2-5(4)15)18-9-3-6(16)10(14)11(17)12(9)19-7/h1-
**InchiKey:** GNJKWCIAEOGLTR-UHFFFAOYSA-N
**Formula:** C12H3Br2Cl3O2
**SMILES:** Clc1cc2c(cc1Br)Oc1c(cc(Cl)c(Br)c1Cl)O2
**Mol. weight [g/mol]:** 445.32

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 108.74 | kJ/mol | Joback Method |
| hf | -57.50 | kJ/mol | Joback Method |
| hfus | 50.48 | kJ/mol | Joback Method |
| hvap | 86.59 | kJ/mol | Joback Method |
| log10ws | -7.37 | | Crippen Method |
| logp | 7.070 | | Crippen Method |
| mcvol | 205.020 | ml/mol | McGowan Method |
| pc | 3602.88 | kPa | Joback Method |
| rinpol | 2582.00 | | NIST Webbook |
| tb | 867.83 | K | Joback Method |
| tc | 1151.65 | K | Joback Method |
| tf | 653.68 | K | Joback Method |
| vc | 0.770 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 414.87 | J/mol×K | 867.83 | Joback Method |
| cpg | 448.08 | J/mol×K | 1104.35 | Joback Method |
| cpg | 441.28 | J/mol×K | 1057.04 | Joback Method |
| cpg | 434.72 | J/mol×K | 1009.74 | Joback Method |
| cpg | 428.23 | J/mol×K | 962.44 | Joback Method |
| cpg | 421.66 | J/mol×K | 915.13 | Joback Method |
| cpg | 455.26 | J/mol×K | 1151.65 | Joback Method |
| dvisc | 0.0003762 | Pa×s | 867.83 | Joback Method |
| dvisc | 0.0004195 | Pa×s | 832.14 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0004724 | Pa×s | 796.45 | Joback Method |
| dvisc | 0.0005379 | Pa×s | 760.76 | Joback Method |
| dvisc | 0.0006203 | Pa×s | 725.06 | Joback Method |
| dvisc | 0.0007260 | Pa×s | 689.37 | Joback Method |
| dvisc | 0.0008645 | Pa×s | 653.68 | Joback Method |

# Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R317374&Units=SI |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |