# octabromodibenzodioxin

**Other names:** Octabromo-dibenzo-p-dioxin
**Inchi:** InChI=1S/C12Br8O2/c13-1-2(14)6(18)10-9(5(1)17)21-11-7(19)3(15)4(16)8(20)12(11)22-1
**InchiKey:** XAHTWKGGNHXJRP-UHFFFAOYSA-N
**Formula:** C12Br8O2
**SMILES:** Brc1c(Br)c(Br)c2c(c1Br)Oc1c(Br)c(Br)c(Br)c(Br)c1O2
**Mol. weight [g/mol]:** 815.36

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 201.56 | kJ/mol | Joback Method |
| hf | 113.29 | kJ/mol | Joback Method |
| hfus | 68.43 | kJ/mol | Joback Method |
| hvap | 114.03 | kJ/mol | Joback Method |
| log10ws | -12.29 | | Crippen Method |
| logp | 9.685 | | Crippen Method |
| mcvol | 273.300 | ml/mol | McGowan Method |
| pc | 7109.36 | kPa | Joback Method |
| rinpol | 4303.00 | | NIST Webbook |
| rinpol | 4303.00 | | NIST Webbook |
| tb | 1167.44 | K | Joback Method |
| tc | 1491.71 | K | Joback Method |
| tf | 960.28 | K | Joback Method |
| vc | 0.996 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 483.89 | J/mol×K | 1167.44 | Joback Method |
| cpg | 575.20 | J/mol×K | 1437.67 | Joback Method |
| cpg | 551.15 | J/mol×K | 1383.62 | Joback Method |
| cpg | 530.33 | J/mol×K | 1329.58 | Joback Method |
| cpg | 512.39 | J/mol×K | 1275.53 | Joback Method |
| cpg | 497.02 | J/mol×K | 1221.49 | Joback Method |
| cpg | 602.80 | J/mol×K | 1491.71 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001253 | Pa×s | 1167.44 | Joback Method |
| dvisc | 0.0001364 | Pa×s | 1132.91 | Joback Method |
| dvisc | 0.0001492 | Pa×s | 1098.39 | Joback Method |
| dvisc | 0.0001643 | Pa×s | 1063.86 | Joback Method |
| dvisc | 0.0001819 | Pa×s | 1029.33 | Joback Method |
| dvisc | 0.0002030 | Pa×s | 994.81 | Joback Method |
| dvisc | 0.0002282 | Pa×s | 960.28 | Joback Method |

# Sources

| | |
|---|---|
| **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=R172240&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **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 |