# Oxetane, 3-bromomethyl-3-(2-chlorophenyloxy)methyl

**Inchi:** InChI=1S/C11H12BrClO2/c12-5-11(6-14-7-11)8-15-10-4-2-1-3-9(10)13/h1-4H,5-8H2

**InchiKey:** GJBLFJPTYOCVOG-UHFFFAOYSA-N

**Formula:** C11H12BrClO2

**SMILES:** Clc1ccccc1OCC1(CBr)COC1

**Mol. weight [g/mol]:** 291.57

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1.05 | kJ/mol | Joback Method |
| hf | -217.06 | kJ/mol | Joback Method |
| hfus | 26.28 | kJ/mol | Joback Method |
| hvap | 59.69 | kJ/mol | Joback Method |
| log10ws | -3.12 | | Crippen Method |
| logp | 3.130 | | Crippen Method |
| mcvol | 172.710 | ml/mol | McGowan Method |
| pc | 3257.86 | kPa | Joback Method |
| rinpol | 1884.00 | | NIST Webbook |
| rinpol | 1884.00 | | NIST Webbook |
| tb | 646.95 | K | Joback Method |
| tc | 896.66 | K | Joback Method |
| tf | 429.51 | K | Joback Method |
| vc | 0.640 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 406.59 | J/mol×K | 646.95 | Joback Method |
| cpg | 420.28 | J/mol×K | 688.57 | Joback Method |
| cpg | 433.12 | J/mol×K | 730.19 | Joback Method |
| cpg | 445.31 | J/mol×K | 771.81 | Joback Method |
| cpg | 457.04 | J/mol×K | 813.42 | Joback Method |
| cpg | 468.52 | J/mol×K | 855.04 | Joback Method |
| cpg | 479.96 | J/mol×K | 896.66 | 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=R6609&Units=SI |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |