# 2-Bromobenzoic acid, 3,4-dichlorophenyl ester

**Inchi:** InChI=1S/C13H7BrCl2O2/c14-10-4-2-1-3-9(10)13(17)18-8-5-6-11(15)12(16)7-8/h1-7H
**InchiKey:** GZDKZNTZGVTCOJ-UHFFFAOYSA-N
**Formula:** C13H7BrCl2O2
**SMILES:** O=C(Oc1ccc(Cl)c(Cl)c1)c1ccccc1Br
**Mol. weight [g/mol]:** 346.00

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 11.05 | kJ/mol | Joback Method |
| hf | -122.95 | kJ/mol | Joback Method |
| hfus | 32.81 | kJ/mol | Joback Method |
| hvap | 75.43 | kJ/mol | Joback Method |
| log10ws | -6.09 | | Crippen Method |
| logp | 4.975 | | Crippen Method |
| mcvol | 195.930 | ml/mol | McGowan Method |
| pc | 3059.17 | kPa | Joback Method |
| rinpol | 2280.00 | | NIST Webbook |
| tb | 782.45 | K | Joback Method |
| tc | 1047.67 | K | Joback Method |
| tf | 518.47 | K | Joback Method |
| vc | 0.732 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 437.33 | J/mol×K | 782.45 | Joback Method |
| cpg | 477.43 | J/mol×K | 1003.47 | Joback Method |
| cpg | 471.21 | J/mol×K | 959.26 | Joback Method |
| cpg | 464.15 | J/mol×K | 915.06 | Joback Method |
| cpg | 456.19 | J/mol×K | 870.86 | Joback Method |
| cpg | 447.27 | J/mol×K | 826.65 | Joback Method |
| cpg | 482.86 | J/mol×K | 1047.67 | Joback Method |
| dvisc | 0.0001248 | Pa×s | 782.45 | Joback Method |
| dvisc | 0.0001503 | Pa×s | 738.45 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001853 | Pa×s | 694.46 | Joback Method |
| dvisc | 0.0002351 | Pa×s | 650.46 | Joback Method |
| dvisc | 0.0003088 | Pa×s | 606.46 | Joback Method |
| dvisc | 0.0004232 | Pa×s | 562.47 | Joback Method |
| dvisc | 0.0006118 | Pa×s | 518.47 | Joback Method |

# Sources

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|---|---|
| **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=U307747&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 |

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