# 3-Bromobenzoic acid, 4-chlorophenyl ester

**Inchi:** InChI=1S/C13H8BrClO2/c14-10-3-1-2-9(8-10)13(16)17-12-6-4-11(15)5-7-12/h1-8H
**InchiKey:** RQRRAGUHQUXGRR-UHFFFAOYSA-N
**Formula:** C13H8BrClO2
**SMILES:** O=C(Oc1ccc(Cl)cc1)c1cccc(Br)c1
**Mol. weight [g/mol]:** 311.56

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 32.61 | kJ/mol | Joback Method |
| hf | -95.74 | kJ/mol | Joback Method |
| hfus | 29.00 | kJ/mol | Joback Method |
| hvap | 70.38 | kJ/mol | Joback Method |
| log10ws | -5.41 | | Crippen Method |
| logp | 4.322 | | Crippen Method |
| mcvol | 183.690 | ml/mol | McGowan Method |
| pc | 3243.03 | kPa | Joback Method |
| rinpol | 2100.00 | | NIST Webbook |
| tb | 740.04 | K | Joback Method |
| tc | 1003.05 | K | Joback Method |
| tf | 476.03 | K | Joback Method |
| vc | 0.682 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 419.51 | J/mol×K | 740.04 | Joback Method |
| cpg | 430.79 | J/mol×K | 783.88 | Joback Method |
| cpg | 440.98 | J/mol×K | 827.71 | Joback Method |
| cpg | 450.16 | J/mol×K | 871.55 | Joback Method |
| cpg | 458.37 | J/mol×K | 915.38 | Joback Method |
| cpg | 465.68 | J/mol×K | 959.22 | Joback Method |
| cpg | 472.17 | J/mol×K | 1003.05 | Joback Method |
| dvisc | 0.0007959 | Pa×s | 476.03 | Joback Method |
| dvisc | 0.0005267 | Pa×s | 520.03 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0003717 | Pa×s | 564.03 | Joback Method |
| dvisc | 0.0002759 | Pa×s | 608.03 | Joback Method |
| dvisc | 0.0002132 | Pa×s | 652.04 | Joback Method |
| dvisc | 0.0001702 | Pa×s | 696.04 | Joback Method |
| dvisc | 0.0001396 | Pa×s | 740.04 | 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=U307549&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 |