# 2-Bromobenzoic acid, 3-methylphenyl ester

**Inchi:** InChI=1S/C14H11BrO2/c1-10-5-4-6-11(9-10)17-14(16)12-7-2-3-8-13(12)15/h2-9H,1H3
**InchiKey:** ZBUIDKJUUGAZSG-UHFFFAOYSA-N
**Formula:** C14H11BrO2
**SMILES:** Cc1cccc(OC(=O)c2ccccc2Br)c1
**Mol. weight [g/mol]:** 291.14

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 52.96 | kJ/mol | Joback Method |
| hf | -100.64 | kJ/mol | Joback Method |
| hfus | 27.39 | kJ/mol | Joback Method |
| hvap | 68.22 | kJ/mol | Joback Method |
| log10ws | -5.20 | | Crippen Method |
| logp | 3.977 | | Crippen Method |
| mcvol | 185.540 | ml/mol | McGowan Method |
| pc | 3035.62 | kPa | Joback Method |
| rinpol | 1991.00 | | NIST Webbook |
| rinpol | 1991.00 | | NIST Webbook |
| tb | 725.49 | K | Joback Method |
| tc | 980.66 | K | Joback Method |
| tf | 457.38 | K | Joback Method |
| vc | 0.690 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 448.93 | J/mol×K | 725.49 | Joback Method |
| cpg | 462.05 | J/mol×K | 768.02 | Joback Method |
| cpg | 474.03 | J/mol×K | 810.55 | Joback Method |
| cpg | 484.93 | J/mol×K | 853.07 | Joback Method |
| cpg | 494.80 | J/mol×K | 895.60 | Joback Method |
| cpg | 503.71 | J/mol×K | 938.13 | Joback Method |
| cpg | 511.71 | J/mol×K | 980.66 | Joback Method |
| dvisc | 0.0008431 | Pa×s | 457.38 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0005446 | Pa×s | 502.06 | Joback Method |
| dvisc | 0.0003778 | Pa×s | 546.75 | Joback Method |
| dvisc | 0.0002770 | Pa×s | 591.43 | Joback Method |
| dvisc | 0.0002121 | Pa×s | 636.12 | Joback Method |
| dvisc | 0.0001683 | Pa×s | 680.81 | Joback Method |
| dvisc | 0.0001373 | Pa×s | 725.49 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U307742&Units=SI |
| **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 |

# 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 |