# 2-Bromobenzoic acid, 3-ethylphenyl ester

**Inchi:** InChI=1S/C15H13BrO2/c1-2-11-6-5-7-12(10-11)18-15(17)13-8-3-4-9-14(13)16/h3-10H,2
**InchiKey:** HSBULRZWONZIRG-UHFFFAOYSA-N
**Formula:** C15H13BrO2
**SMILES:** CCc1cccc(OC(=O)c2ccccc2Br)c1
**Mol. weight [g/mol]:** 305.17

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 61.38 | kJ/mol | Joback Method |
| hf | -121.28 | kJ/mol | Joback Method |
| hfus | 29.98 | kJ/mol | Joback Method |
| hvap | 70.45 | kJ/mol | Joback Method |
| log10ws | -5.52 | | Crippen Method |
| logp | 4.231 | | Crippen Method |
| mcvol | 199.630 | ml/mol | McGowan Method |
| pc | 2738.28 | kPa | Joback Method |
| rinpol | 2196.00 | | NIST Webbook |
| rinpol | 2196.00 | | NIST Webbook |
| tb | 748.37 | K | Joback Method |
| tc | 997.92 | K | Joback Method |
| tf | 468.65 | K | Joback Method |
| vc | 0.746 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 500.84 | J/mol×K | 748.37 | Joback Method |
| cpg | 557.83 | J/mol×K | 956.33 | Joback Method |
| cpg | 548.50 | J/mol×K | 914.73 | Joback Method |
| cpg | 538.20 | J/mol×K | 873.14 | Joback Method |
| cpg | 526.86 | J/mol×K | 831.55 | Joback Method |
| cpg | 514.43 | J/mol×K | 789.96 | Joback Method |
| cpg | 566.25 | J/mol×K | 997.92 | Joback Method |
| dvisc | 0.0001217 | Pa×s | 748.37 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001498 | Pa×s | 701.75 | Joback Method |
| dvisc | 0.0001899 | Pa×s | 655.13 | Joback Method |
| dvisc | 0.0002497 | Pa×s | 608.51 | Joback Method |
| dvisc | 0.0003435 | Pa×s | 561.89 | Joback Method |
| dvisc | 0.0005008 | Pa×s | 515.27 | Joback Method |
| dvisc | 0.0007868 | Pa×s | 468.65 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U354676&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 |

# 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 |