

4-Bromophenol, isoBOC

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|-----------------------------|---|
| Inchi: | InChI=1S/C11H13BrO3/c1-8(2)7-14-11(13)15-10-5-3-9(12)4-6-10/h3-6,8H,7H2,1-2H3 |
| InchiKey: | BJLRPRWZWOGQSZ-UHFFFAOYSA-N |
| Formula: | C11H13BrO3 |
| SMILES: | CC(C)COC(=O)Oc1ccc(Br)cc1 |
| Mol. weight [g/mol]: | 273.12 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -182.52 | kJ/mol | Joback Method |
| hf | -401.28 | kJ/mol | Joback Method |
| hfus | 23.64 | kJ/mol | Joback Method |
| hvap | 60.63 | kJ/mol | Joback Method |
| log10ws | -4.03 | | Crippen Method |
| logp | 3.620 | | Crippen Method |
| mvol | 172.900 | ml/mol | McGowan Method |
| pc | 2915.53 | kPa | Joback Method |
| rmpol | 1652.00 | | NIST Webbook |
| tb | 647.17 | K | Joback Method |
| tc | 871.68 | K | Joback Method |
| tf | 391.86 | K | Joback Method |
| vc | 0.641 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 409.45 | J/molxK | 647.17 | Joback Method |
| cpg | 422.58 | J/molxK | 684.59 | Joback Method |
| cpg | 434.86 | J/molxK | 722.01 | Joback Method |
| cpg | 446.32 | J/molxK | 759.42 | Joback Method |
| cpg | 456.95 | J/molxK | 796.84 | Joback Method |
| cpg | 466.78 | J/molxK | 834.26 | Joback Method |
| cpg | 475.81 | J/molxK | 871.68 | Joback Method |
| dvisc | 0.0012047 | Paxs | 391.86 | Joback Method |
| dvisc | 0.0007054 | Paxs | 434.41 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0004544 | Paxs | 476.96 | Joback Method |
| dvisc | 0.0003146 | Paxs | 519.52 | Joback Method |
| dvisc | 0.0002303 | Paxs | 562.07 | Joback Method |
| dvisc | 0.0001761 | Paxs | 604.62 | Joback Method |
| dvisc | 0.0001395 | Paxs | 647.17 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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=R235168&Units=SI |

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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