# Bromo STP

**Inchi:** InChI=1S/C11H16BrNO2/c1-7-9(14-2)6-8(4-5-13)11(15-3)10(7)12/h6H,4-5,13H2,1-3H3
**InchiKey:** CFNPHYJWDYQUCU-UHFFFAOYSA-N
**Formula:** C11H16BrNO2
**SMILES:** COc1cc(CCN)c(OC)c(Br)c1C
**Mol. weight [g/mol]:** 274.15

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -13.60 | kJ/mol | Joback Method |
| hf | -284.04 | kJ/mol | Joback Method |
| hfus | 29.59 | kJ/mol | Joback Method |
| hvap | 66.90 | kJ/mol | Joback Method |
| log10ws | -3.59 | | Crippen Method |
| logp | 2.276 | | Crippen Method |
| mcvol | 181.310 | ml/mol | McGowan Method |
| pc | 2738.28 | kPa | Joback Method |
| rinpol | 2195.00 | | NIST Webbook |
| rinpol | 2195.00 | | NIST Webbook |
| rinpol | 2195.00 | | NIST Webbook |
| tb | 681.21 | K | Joback Method |
| tc | 904.00 | K | Joback Method |
| tf | 477.75 | K | Joback Method |
| vc | 0.670 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 449.66 | J/mol×K | 681.21 | Joback Method |
| cpg | 462.85 | J/mol×K | 718.34 | Joback Method |
| cpg | 475.30 | J/mol×K | 755.47 | Joback Method |
| cpg | 486.99 | J/mol×K | 792.60 | Joback Method |
| cpg | 497.93 | J/mol×K | 829.73 | Joback Method |
| cpg | 508.10 | J/mol×K | 866.87 | Joback Method |
| cpg | 517.50 | J/mol×K | 904.00 | Joback Method |

# Sources

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|---|---|
| **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=R17234&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |