# Benzamide, N-(4-bromophenyl)-2-methoxy-

**Inchi:** InChI=1S/C14H12BrNO2/c1-18-13-5-3-2-4-12(13)14(17)16-11-8-6-10(15)7-9-11/h2-9H,1
**InchiKey:** JSCDVENNYSRBMK-UHFFFAOYSA-N
**Formula:** C14H12BrNO2
**SMILES:** COc1ccccc1C(=O)Nc1ccc(Br)cc1
**Mol. weight [g/mol]:** 306.15

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 142.35 | kJ/mol | Joback Method |
| hf | -47.17 | kJ/mol | Joback Method |
| hfus | 32.49 | kJ/mol | Joback Method |
| hvap | 74.66 | kJ/mol | Joback Method |
| log10ws | -4.73 | | Crippen Method |
| logp | 3.710 | | Crippen Method |
| mcvol | 195.520 | ml/mol | McGowan Method |
| pc | 3079.57 | kPa | Joback Method |
| rinpol | 2477.00 | | NIST Webbook |
| tb | 775.66 | K | Joback Method |
| tc | 1026.95 | K | Joback Method |
| tf | 510.04 | K | Joback Method |
| vc | 0.725 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 497.84 | J/mol×K | 775.66 | Joback Method |
| cpg | 510.24 | J/mol×K | 817.54 | Joback Method |
| cpg | 521.51 | J/mol×K | 859.42 | Joback Method |
| cpg | 531.73 | J/mol×K | 901.31 | Joback Method |
| cpg | 540.94 | J/mol×K | 943.19 | Joback Method |
| cpg | 549.22 | J/mol×K | 985.07 | Joback Method |
| cpg | 556.61 | J/mol×K | 1026.95 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U307061&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 |
| **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 |