# Benzamide, 3-bromo-N-butyl-N-methyl-

**Inchi:** InChI=1S/C12H16BrNO/c1-3-4-8-14(2)12(15)10-6-5-7-11(13)9-10/h5-7,9H,3-4,8H2,1-2H
**InchiKey:** UZZYLLYPEJVLDE-UHFFFAOYSA-N
**Formula:** C12H16BrNO
**SMILES:** CCCCN(C)C(=O)c1cccc(Br)c1
**Mol. weight [g/mol]:** 270.17

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 149.12 | kJ/mol | Joback Method |
| hf | -84.67 | kJ/mol | Joback Method |
| hfus | 30.39 | kJ/mol | Joback Method |
| hvap | 60.47 | kJ/mol | Joback Method |
| log10ws | -4.03 | | Crippen Method |
| logp | 3.321 | | Crippen Method |
| mcvol | 185.230 | ml/mol | McGowan Method |
| pc | 2701.41 | kPa | Joback Method |
| rinpol | 2206.00 | | NIST Webbook |
| tb | 638.09 | K | Joback Method |
| tc | 856.52 | K | Joback Method |
| tf | 406.14 | K | Joback Method |
| vc | 0.685 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 446.12 | J/mol×K | 638.09 | Joback Method |
| cpg | 460.52 | J/mol×K | 674.49 | Joback Method |
| cpg | 473.96 | J/mol×K | 710.90 | Joback Method |
| cpg | 486.48 | J/mol×K | 747.30 | Joback Method |
| cpg | 498.15 | J/mol×K | 783.71 | Joback Method |
| cpg | 509.03 | J/mol×K | 820.11 | Joback Method |
| cpg | 519.16 | J/mol×K | 856.52 | 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=U415656&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 |
| **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 |