# Benzamide, N-ethyl-N-(3-methylphenyl)-4-bromo-

**Inchi:** InChI=1S/C16H16BrNO/c1-3-18(15-6-4-5-12(2)11-15)16(19)13-7-9-14(17)10-8-13/h4-11

**InchiKey:** NXRHHDOCCGXWJH-UHFFFAOYSA-N

**Formula:** C16H16BrNO

**SMILES:** CCN(C(=O)c1ccc(Br)cc1)c1cccc(C)c1

**Mol. weight [g/mol]:** 318.21

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 285.58 | kJ/mol | Joback Method |
| hf | 57.83 | kJ/mol | Joback Method |
| hfus | 34.40 | kJ/mol | Joback Method |
| hvap | 72.31 | kJ/mol | Joback Method |
| log10ws | -5.40 | | Crippen Method |
| logp | 4.424 | | Crippen Method |
| mcvol | 217.830 | ml/mol | McGowan Method |
| pc | 2520.12 | kPa | Joback Method |
| rinpol | 2119.00 | | NIST Webbook |
| rinpol | 2119.00 | | NIST Webbook |
| tb | 761.27 | K | Joback Method |
| tc | 1005.54 | K | Joback Method |
| tf | 490.16 | K | Joback Method |
| vc | 0.801 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 567.67 | J/mol×K | 761.27 | Joback Method |
| cpg | 582.19 | J/mol×K | 801.98 | Joback Method |
| cpg | 595.52 | J/mol×K | 842.69 | Joback Method |
| cpg | 607.78 | J/mol×K | 883.41 | Joback Method |
| cpg | 619.05 | J/mol×K | 924.12 | Joback Method |
| cpg | 629.43 | J/mol×K | 964.83 | Joback Method |
| cpg | 639.04 | J/mol×K | 1005.54 | 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=U308452&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 |