# Benzamide, 2-bromo-N-ethyl-N-octadecyl-

**Inchi:** InChI=1S/C27H46BrNO/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-24-29(4-2)27(30
**InchiKey:** OHNLLTNBGWHSCN-UHFFFAOYSA-N
**Formula:** C27H46BrNO
**SMILES:** CCCCCCCCCCCCCCCCCCN(CC)C(=O)c1ccccc1Br
**Mol. weight [g/mol]:** 480.56

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 275.42 | kJ/mol | Joback Method |
| hf | -394.27 | kJ/mol | Joback Method |
| hfus | 69.24 | kJ/mol | Joback Method |
| hvap | 93.86 | kJ/mol | Joback Method |
| log10ws | -10.31 | | Crippen Method |
| logp | 9.173 | | Crippen Method |
| mcvol | 396.580 | ml/mol | McGowan Method |
| pc | 883.67 | kPa | Joback Method |
| rinpol | 1710.00 | | NIST Webbook |
| rinpol | 1710.00 | | NIST Webbook |
| tb | 981.29 | K | Joback Method |
| tc | 1201.73 | K | Joback Method |
| tf | 575.19 | K | Joback Method |
| vc | 1.526 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1316.66 | J/mol×K | 981.29 | Joback Method |
| cpg | 1336.34 | J/mol×K | 1018.03 | Joback Method |
| cpg | 1354.84 | J/mol×K | 1054.77 | Joback Method |
| cpg | 1372.28 | J/mol×K | 1091.51 | Joback Method |
| cpg | 1388.77 | J/mol×K | 1128.25 | Joback Method |
| cpg | 1404.41 | J/mol×K | 1164.99 | Joback Method |
| cpg | 1419.33 | J/mol×K | 1201.73 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U415370&Units=SI |

# 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 |