# Benzamide, n,n-didecyl-3-bromo-

**Inchi:** InChI=1S/C27H46BrNO/c1-3-5-7-9-11-13-15-17-22-29(23-18-16-14-12-10-8-6-4-2)27(30
**InchiKey:** WXMVNEJSALHXED-UHFFFAOYSA-N
**Formula:** C27H46BrNO
**SMILES:** CCCCCCCCCCN(CCCCCCCCCC)C(=O)c1cccc(Br)c1
**Mol. weight [g/mol]:** 480.57

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -473.80 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 69.24 | kJ/mol | Joback Method |
| hvap | 125.02 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.66 | eV | Cheméo Relay (1.0) |
| log10ws | -8.79 | | Cheméo Relay (1.0) |
| logp | 9.173 | | Crippen Method |
| mcvol | 396.580 | ml/mol | McGowan Method |
| rinpol | 3246.00 | | NIST Webbook |
| rinpol | 3246.00 | | NIST Webbook |
| tb | 703.24 | K | Cheméo Relay (1.0) |
| tf | 314.46 | K | Cheméo Relay (1.0) |

## 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

| | |
|---|---|
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U308629&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tf:** | Normal melting (fusion) point |