

Benzamide, 4-methyl-N-butyl-N-3-methylbutyl-

| | |
|-----------------------------|--|
| Inchi: | InChI=1S/C17H27NO/c1-5-6-12-18(13-11-14(2)3)17(19)16-9-7-15(4)8-10-16/h7-10,14H, |
| InchiKey: | HCBPIUBKKLKLI-UHFFFAOYSA-N |
| Formula: | C17H27NO |
| SMILES: | CCCCN(CCC(C)C)C(=O)c1ccc(C)cc1 |
| Mol. weight [g/mol]: | 261.40 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 174.46 | kJ/mol | Joback Method |
| hf | -219.48 | kJ/mol | Joback Method |
| hfus | 34.53 | kJ/mol | Joback Method |
| hvap | 64.78 | kJ/mol | Joback Method |
| log10ws | -4.78 | | Crippen Method |
| logp | 4.283 | | Crippen Method |
| mvol | 238.180 | ml/mol | McGowan Method |
| pc | 1645.76 | kPa | Joback Method |
| rinpol | 2452.00 | | NIST Webbook |
| rinpol | 2452.00 | | NIST Webbook |
| tb | 685.89 | K | Joback Method |
| tc | 882.46 | K | Joback Method |
| tf | 387.69 | K | Joback Method |
| vc | 0.897 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 666.24 | J/mol×K | 685.89 | Joback Method |
| cpg | 684.45 | J/mol×K | 718.65 | Joback Method |
| cpg | 701.60 | J/mol×K | 751.41 | Joback Method |
| cpg | 717.75 | J/mol×K | 784.18 | Joback Method |
| cpg | 732.95 | J/mol×K | 816.94 | Joback Method |
| cpg | 747.23 | J/mol×K | 849.70 | Joback Method |
| cpg | 760.65 | J/mol×K | 882.46 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U415922&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.cheméo.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

| | |
|-----------------|---|
| 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 |
| hvp: | 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 |
| rinp: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

Latest version available from:

<https://www.cheméo.com/cid/90-398-1/Benzamide-4-methyl-N-butyl-N-3-methylbutyl.pdf>

Generated by Cheméo on 2024-04-19 01:55:13.711399501 +0000 UTC m=+15780962.631976817.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.