

Cyclopentanecarboxamide, N-butyl-N-methyl-

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|-----------------------------|--|
| Inchi: | InChI=1S/C11H21NO/c1-3-4-9-12(2)11(13)10-7-5-6-8-10/h10H,3-9H2,1-2H3 |
| InchiKey: | ILYRBGWZFLTSSQ-UHFFFAOYSA-N |
| Formula: | C11H21NO |
| SMILES: | CCCCN(C)C(=O)C1CCCC1 |
| Mol. weight [g/mol]: | 183.29 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 60.15 | kJ/mol | Joback Method |
| hf | -254.94 | kJ/mol | Joback Method |
| hfus | 22.80 | kJ/mol | Joback Method |
| hvap | 49.13 | kJ/mol | Joback Method |
| log10ws | -2.43 | | Crippen Method |
| logp | 2.435 | | Crippen Method |
| mcvol | 166.540 | ml/mol | McGowan Method |
| pc | 2419.50 | kPa | Joback Method |
| rinpol | 1645.00 | | NIST Webbook |
| rinpol | 1645.00 | | NIST Webbook |
| tb | 532.67 | K | Joback Method |
| tc | 727.28 | K | Joback Method |
| tf | 307.03 | K | Joback Method |
| vc | 0.617 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 411.52 | J/mol×K | 532.67 | Joback Method |
| cpg | 430.08 | J/mol×K | 565.10 | Joback Method |
| cpg | 447.63 | J/mol×K | 597.54 | Joback Method |
| cpg | 464.22 | J/mol×K | 629.97 | Joback Method |
| cpg | 479.88 | J/mol×K | 662.41 | Joback Method |
| cpg | 494.65 | J/mol×K | 694.84 | Joback Method |
| cpg | 508.57 | J/mol×K | 727.28 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=U415623&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |

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.chemeo.com/cid/82-784-1/Cyclopentanecarboxamide-N-butyl-N-methyl.pdf>

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