

Cyclopentanecarboxamide, N,N-dinonyl-

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|-----------------------------|---|
| Inchi: | InChI=1S/C24H47NO/c1-3-5-7-9-11-13-17-21-25(24(26)23-19-15-16-20-23)22-18-14-12 |
| InchiKey: | KFEFBVCGNYGRQS-UHFFFAOYSA-N |
| Formula: | C24H47NO |
| SMILES: | CCCCCCCCCN(CCCCCCCC)C(=O)C1CCCC1 |
| Mol. weight [g/mol]: | 365.64 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 169.61 | kJ/mol | Joback Method |
| hf | -523.26 | kJ/mol | Joback Method |
| hfus | 56.47 | kJ/mol | Joback Method |
| hvap | 78.06 | kJ/mol | Joback Method |
| log10ws | -7.87 | | Crippen Method |
| logp | 7.506 | | Crippen Method |
| mvol | 349.710 | ml/mol | McGowan Method |
| pc | 928.94 | kPa | Joback Method |
| rinpol | 2577.00 | | NIST Webbook |
| rinpol | 2577.00 | | NIST Webbook |
| tb | 830.11 | K | Joback Method |
| tc | 1018.79 | K | Joback Method |
| tf | 453.54 | K | Joback Method |
| vc | 1.345 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|---------|---------|-----------------|---------------|
| cpg | 1162.05 | J/mol×K | 830.11 | Joback Method |
| cpg | 1184.16 | J/mol×K | 861.56 | Joback Method |
| cpg | 1205.06 | J/mol×K | 893.00 | Joback Method |
| cpg | 1224.80 | J/mol×K | 924.45 | Joback Method |
| cpg | 1243.44 | J/mol×K | 955.90 | Joback Method |
| cpg | 1261.05 | J/mol×K | 987.34 | Joback Method |
| cpg | 1277.69 | J/mol×K | 1018.79 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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=U308616&Units=SI |

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/86-827-9/Cyclopentanecarboxamide-N-N-dinonyl.pdf>

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