

Propanamide, N,N-didecyl-3-cyclopentyl-

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|-----------------------------|--|
| Inchi: | InChI=1S/C28H55NO/c1-3-5-7-9-11-13-15-19-25-29(26-20-16-14-12-10-8-6-4-2)28(30)2 |
| InchiKey: | KWSXWJUPXHUAHC-UHFFFAOYSA-N |
| Formula: | C28H55NO |
| SMILES: | CCCCCCCCCN(CCCCCCCCCC)C(=O)CCC1CCCC1 |
| Mol. weight [g/mol]: | 421.74 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 203.29 | kJ/mol | Joback Method |
| hf | -605.82 | kJ/mol | Joback Method |
| hfus | 66.83 | kJ/mol | Joback Method |
| hvap | 86.97 | kJ/mol | Joback Method |
| log10ws | -9.54 | | Crippen Method |
| logp | 9.067 | | Crippen Method |
| mcvol | 406.070 | ml/mol | McGowan Method |
| pc | 744.48 | kPa | Joback Method |
| rinpol | 3138.00 | | NIST Webbook |
| rinpol | 3138.00 | | NIST Webbook |
| tb | 921.63 | K | Joback Method |
| tc | 1129.65 | K | Joback Method |
| tf | 498.62 | K | Joback Method |
| vc | 1.569 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|---------|---------|-----------------|---------------|
| cpg | 1422.09 | J/mol×K | 921.63 | Joback Method |
| cpg | 1446.06 | J/mol×K | 956.30 | Joback Method |
| cpg | 1468.58 | J/mol×K | 990.97 | Joback Method |
| cpg | 1489.75 | J/mol×K | 1025.64 | Joback Method |
| cpg | 1509.67 | J/mol×K | 1060.31 | Joback Method |
| cpg | 1528.43 | J/mol×K | 1094.98 | Joback Method |
| cpg | 1546.14 | J/mol×K | 1129.65 | 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=U308288&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 |
| 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 |
| rinpola: | 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/87-868-3/Propanamide-N-N-didecyl-3-cyclopentyl.pdf>

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