

Octanamide, N-heptyl-N-octyl-

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|-----------------------------|--|
| Inchi: | InChI=1S/C23H47NO/c1-4-7-10-13-16-19-22-24(21-18-15-12-9-6-3)23(25)20-17-14-11-8 |
| InchiKey: | VDKVPXDTTYCOCO-UHFFFAOYSA-N |
| Formula: | C23H47NO |
| SMILES: | CCCCCCCCN(CCCCCC)C(=O)CCCCC |
| Mol. weight [g/mol]: | 353.63 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 124.64 | kJ/mol | Joback Method |
| hf | -563.10 | kJ/mol | Joback Method |
| hfus | 59.95 | kJ/mol | Joback Method |
| hvap | 75.58 | kJ/mol | Joback Method |
| log10ws | -7.80 | | Crippen Method |
| logp | 7.506 | | Crippen Method |
| mvol | 346.480 | ml/mol | McGowan Method |
| pc | 883.14 | kPa | Joback Method |
| rinpol | 2493.00 | | NIST Webbook |
| tb | 791.95 | K | Joback Method |
| tc | 970.38 | K | Joback Method |
| tf | 431.37 | K | Joback Method |
| vc | 1.347 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|---------|---------|-----------------|---------------|
| cpg | 1103.84 | J/molxK | 791.95 | Joback Method |
| cpg | 1125.27 | J/molxK | 821.69 | Joback Method |
| cpg | 1145.63 | J/molxK | 851.43 | Joback Method |
| cpg | 1164.98 | J/molxK | 881.17 | Joback Method |
| cpg | 1183.34 | J/molxK | 910.91 | Joback Method |
| cpg | 1200.78 | J/molxK | 940.65 | Joback Method |
| cpg | 1217.32 | J/molxK | 970.38 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=U308445&Units=SI |
| 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 |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| h vap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| m cvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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