

1,3-Dicyclohexylurea

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|-----------------------------|---|
| Other names: | Urea, N,N'-dicyclohexyl- Urea, 1,3-dicyclohexyl- N,N'-Dicyclohexylurea |
| Inchi: | InChI=1S/C13H24N2O/c16-13(14-11-7-3-1-4-8-11)15-12-9-5-2-6-10-12/h11-12H,1-10H2 |
| InchiKey: | ADFXKUOMJKEIND-UHFFFAOYSA-N |
| Formula: | C13H24N2O |
| SMILES: | O=C(NC1CCCCC1)NC1CCCCC1 |
| Mol. weight [g/mol]: | 224.34 |
| CAS: | 2387-23-7 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 157.34 | kJ/mol | Joback Method |
| hf | -208.65 | kJ/mol | Joback Method |
| hfus | 24.89 | kJ/mol | Joback Method |
| hvap | 65.01 | kJ/mol | Joback Method |
| log10ws | -4.41 | | Crippen Method |
| logp | 2.951 | | Crippen Method |
| mcvol | 193.840 | ml/mol | McGowan Method |
| pc | 2584.59 | kPa | Joback Method |
| tb | 690.15 | K | Joback Method |
| tc | 921.88 | K | Joback Method |
| tf | 406.28 | K | Joback Method |
| vc | 0.706 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 591.50 | J/molxK | 690.15 | Joback Method |
| cpg | 613.14 | J/molxK | 728.77 | Joback Method |
| cpg | 633.16 | J/molxK | 767.39 | Joback Method |
| cpg | 651.63 | J/molxK | 806.02 | Joback Method |
| cpg | 668.59 | J/molxK | 844.64 | Joback Method |
| cpg | 684.13 | J/molxK | 883.26 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C2387237&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| 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 |

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 |
| mccvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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