

Propanamide, N-hexyl-2,2-dimethyl

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|-----------------------------|---|
| Inchi: | InChI=1S/C11H23NO/c1-5-6-7-8-9-12-10(13)11(2,3)4/h5-9H2,1-4H3,(H,12,13) |
| InchiKey: | BMBYFLMIWBXBIV-UHFFFAOYSA-N |
| Formula: | C11H23NO |
| SMILES: | CCCCCN=C(O)C(C)(C)C |
| Mol. weight [g/mol]: | 185.31 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | -358.92 | kJ/mol | Joback Method |
| hvap | 58.86 | kJ/mol | Joback Method |
| log10ws | -3.17 | | Crippen Method |
| logp | 3.569 | | Crippen Method |
| mcvol | 177.400 | ml/mol | McGowan Method |
| pc | 1952.68 | kPa | Joback Method |
| rinpol | 1386.00 | | NIST Webbook |
| rinpol | 1386.00 | | NIST Webbook |
| tb | 616.59 | K | Joback Method |
| tc | 799.54 | K | 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=R50903&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |

Legend

| | |
|--------------|---|
| hf: | Enthalpy of formation 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 |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |

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