

Propanamide, 3-phenyl-N-hexyl-

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|-----------------------------|---|
| Inchi: | InChI=1S/C15H23NO/c1-2-3-4-8-13-16-15(17)12-11-14-9-6-5-7-10-14/h5-7,9-10H,2-4,8, |
| InchiKey: | QYYCHRTXCLGUEZ-UHFFFAOYSA-N |
| Formula: | C15H23NO |
| SMILES: | CCCCCN=C(O)CCc1ccccc1 |
| Mol. weight [g/mol]: | 233.35 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | -196.20 | kJ/mol | Joback Method |
| hvap | 71.33 | kJ/mol | Joback Method |
| log10ws | -4.19 | | Crippen Method |
| logp | 4.156 | | Crippen Method |
| mcvol | 210.000 | ml/mol | McGowan Method |
| pc | 1834.11 | kPa | Joback Method |
| rinsol | 2037.00 | | NIST Webbook |
| tb | 738.02 | K | Joback Method |
| tc | 936.48 | K | 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=U407154&Units=SI |

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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