# Propanamide, 3-phenyl-N-(hept-2-yl)-

**Inchi:** InChI=1S/C16H25NO/c1-3-4-6-9-14(2)17-16(18)13-12-15-10-7-5-8-11-15/h5,7-8,10-11,1
**InchiKey:** CSYFFIFXPDNJIH-UHFFFAOYSA-N
**Formula:** C16H25NO
**SMILES:** CCCCCC(C)N=C(O)CCc1ccccc1
**Mol. weight [g/mol]:** 247.38

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -222.12 | kJ/mol | Joback Method |
| hvap | 73.17 | kJ/mol | Joback Method |
| log10ws | -4.72 | | Crippen Method |
| logp | 4.545 | | Crippen Method |
| mcvol | 224.090 | ml/mol | McGowan Method |
| pc | 1703.31 | kPa | Joback Method |
| rinpol | 2012.00 | | NIST Webbook |
| rinpol | 2012.00 | | NIST Webbook |
| tb | 760.46 | K | Joback Method |
| tc | 960.33 | K | Joback Method |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U407153&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

**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 |