# Propanamide, 3-phenyl-N-ethyl-N-butyl-

**Inchi:** InChI=1S/C15H23NO/c1-3-5-13-16(4-2)15(17)12-11-14-9-7-6-8-10-14/h6-10H,3-5,11-13
**InchiKey:** KLMCBOHERMDZAN-UHFFFAOYSA-N
**Formula:** C15H23NO
**SMILES:** CCCCN(CC)C(=O)CCc1ccccc1
**Mol. weight [g/mol]:** 233.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 169.69 | kJ/mol | Joback Method |
| hf | -161.45 | kJ/mol | Joback Method |
| hfus | 33.27 | kJ/mol | Joback Method |
| hvap | 60.05 | kJ/mol | Joback Method |
| log10ws | -3.55 | | Crippen Method |
| logp | 3.268 | | Crippen Method |
| mcvol | 210.000 | ml/mol | McGowan Method |
| pc | 1947.51 | kPa | Joback Method |
| rinpol | 2033.00 | | NIST Webbook |
| tb | 635.59 | K | Joback Method |
| tc | 832.38 | K | Joback Method |
| tf | 367.63 | K | Joback Method |
| vc | 0.791 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 557.20 | J/mol×K | 635.59 | Joback Method |
| cpg | 574.64 | J/mol×K | 668.39 | Joback Method |
| cpg | 591.06 | J/mol×K | 701.19 | Joback Method |
| cpg | 606.51 | J/mol×K | 733.98 | Joback Method |
| cpg | 621.04 | J/mol×K | 766.78 | Joback Method |
| cpg | 634.68 | J/mol×K | 799.58 | Joback Method |
| cpg | 647.49 | J/mol×K | 832.38 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U415392&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

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|---|---|
| **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 |
| **mcvol:** | 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 |