# N-Benzoyl-D-phenylalanine

**Inchi:** InChI=1S/C16H15NO3/c18-15(13-9-5-2-6-10-13)17-14(16(19)20)11-12-7-3-1-4-8-12/h1-1
**InchiKey:** NPKISZUVEBESJI-CQSZACIVSA-N
**Formula:** C16H15NO3
**SMILES:** O=C(NC(Cc1ccccc1)C(=O)O)c1ccccc1
**Mol. weight [g/mol]:** 269.30
**CAS:** 37002-52-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -7936.60 | kJ/mol | NIST Webbook |
| gf | 0.95 | kJ/mol | Joback Method |
| hf | -229.71 | kJ/mol | Joback Method |
| hfus | 34.14 | kJ/mol | Joback Method |
| hvap | 91.98 | kJ/mol | Joback Method |
| log10ws | -3.48 | | Crippen Method |
| logp | 2.112 | | Crippen Method |
| mcvol | 207.770 | ml/mol | McGowan Method |
| pc | 2912.39 | kPa | Joback Method |
| tb | 868.49 | K | Joback Method |
| tc | 1096.36 | K | Joback Method |
| tf | 521.26 | K | Joback Method |
| vc | 0.775 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 608.70 | J/mol×K | 868.49 | Joback Method |
| cpg | 619.38 | J/mol×K | 906.47 | Joback Method |
| cpg | 629.13 | J/mol×K | 944.45 | Joback Method |
| cpg | 638.02 | J/mol×K | 982.43 | Joback Method |
| cpg | 646.14 | J/mol×K | 1020.40 | Joback Method |
| cpg | 653.55 | J/mol×K | 1058.38 | Joback Method |
| cpg | 660.33 | J/mol×K | 1096.36 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C37002521&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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|---|---|
| **chs:** | Standard solid enthalpy of combustion |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |