# Propionamide, 3-benzoyl-

**Inchi:** InChI=1S/C10H11NO2/c11-10(13)7-6-9(12)8-4-2-1-3-5-8/h1-5H,6-7H2,(H2,11,13)
**InchiKey:** PNPJKWAGJXUHIQ-UHFFFAOYSA-N
**Formula:** C10H11NO2
**SMILES:** NC(=O)CCC(=O)c1ccccc1
**Mol. weight [g/mol]:** 177.20
**CAS:** 23132-29-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -45.66 | kJ/mol | Joback Method |
| hf | -204.57 | kJ/mol | Joback Method |
| hfus | 24.09 | kJ/mol | Joback Method |
| hvap | 64.26 | kJ/mol | Joback Method |
| log10ws | -2.18 | | Crippen Method |
| logp | 1.135 | | Crippen Method |
| mcvol | 141.120 | ml/mol | McGowan Method |
| pc | 3611.55 | kPa | Joback Method |
| tb | 635.15 | K | Joback Method |
| tc | 866.24 | K | Joback Method |
| tf | 412.00 | K | Joback Method |
| vc | 0.528 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 348.02 | J/mol×K | 635.15 | Joback Method |
| cpg | 360.09 | J/mol×K | 673.66 | Joback Method |
| cpg | 371.27 | J/mol×K | 712.18 | Joback Method |
| cpg | 381.59 | J/mol×K | 750.69 | Joback Method |
| cpg | 391.10 | J/mol×K | 789.21 | Joback Method |
| cpg | 399.85 | J/mol×K | 827.72 | Joback Method |
| cpg | 407.87 | J/mol×K | 866.24 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C23132298&Units=SI |

# Legend

| | |
|---|---|
| **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 |