# «beta»-Alanine, N-acryloyl-, butyl ester

**Inchi:** InChI=1S/C10H17NO3/c1-3-5-8-14-10(13)6-7-11-9(12)4-2/h4H,2-3,5-8H2,1H3,(H,11,12)
**InchiKey:** JPICICRJSFKZQY-UHFFFAOYSA-N
**Formula:** C10H17NO3
**SMILES:** C=CC(=O)NCCC(=O)OCCCC
**Mol. weight [g/mol]:** 199.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -152.29 | kJ/mol | Joback Method |
| hf | -428.21 | kJ/mol | Joback Method |
| hfus | 29.86 | kJ/mol | Joback Method |
| hvap | 59.52 | kJ/mol | Joback Method |
| log10ws | -1.69 | | Crippen Method |
| logp | 1.022 | | Crippen Method |
| mcvol | 166.450 | ml/mol | McGowan Method |
| pc | 2465.36 | kPa | Joback Method |
| rinpol | 1578.00 | | NIST Webbook |
| rinpol | 1578.00 | | NIST Webbook |
| tb | 605.21 | K | Joback Method |
| tc | 791.03 | K | Joback Method |
| tf | 375.45 | K | Joback Method |
| vc | 0.641 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 420.50 | J/mol×K | 605.21 | Joback Method |
| cpg | 433.30 | J/mol×K | 636.18 | Joback Method |
| cpg | 445.47 | J/mol×K | 667.15 | Joback Method |
| cpg | 457.04 | J/mol×K | 698.12 | Joback Method |
| cpg | 468.00 | J/mol×K | 729.09 | Joback Method |
| cpg | 478.38 | J/mol×K | 760.06 | Joback Method |
| cpg | 488.19 | J/mol×K | 791.03 | Joback Method |

# Sources

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|---|---|
| **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=U321677&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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