

«beta»-Alanine, N-allyloxycarbonyl-, allyl ester

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|-----------------------------|---|
| Inchi: | InChI=1S/C10H15NO4/c1-3-7-14-9(12)5-6-11-10(13)15-8-4-2/h3-4H,1-2,5-8H2,(H,11,13) |
| InchiKey: | ZLTGULSGHUHBNZ-UHFFFAOYSA-N |
| Formula: | C10H15NO4 |
| SMILES: | C=CCOC(=O)CCNC(=O)OCC=C |
| Mol. weight [g/mol]: | 213.23 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -169.45 | kJ/mol | Joback Method |
| hf | -435.00 | kJ/mol | Joback Method |
| hfus | 29.77 | kJ/mol | Joback Method |
| hvap | 61.26 | kJ/mol | Joback Method |
| log10ws | -1.61 | | Crippen Method |
| logp | 1.018 | | Crippen Method |
| mcvol | 168.020 | ml/mol | McGowan Method |
| pc | 2527.73 | kPa | Joback Method |
| rinsol | 1542.00 | | NIST Webbook |
| tb | 624.31 | K | Joback Method |
| tc | 812.20 | K | Joback Method |
| tf | 395.92 | K | Joback Method |
| vc | 0.640 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 424.26 | J/mol×K | 624.31 | Joback Method |
| cpg | 436.29 | J/mol×K | 655.62 | Joback Method |
| cpg | 447.72 | J/mol×K | 686.94 | Joback Method |
| cpg | 458.56 | J/mol×K | 718.25 | Joback Method |
| cpg | 468.81 | J/mol×K | 749.57 | Joback Method |
| cpg | 478.48 | J/mol×K | 780.88 | Joback Method |
| cpg | 487.56 | J/mol×K | 812.20 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| 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=U321033&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 |
| rinpola: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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<https://www.chemeo.com/cid/34-877-1/beta-Alanine-N-allyloxycarbonyl-allyl-ester.pdf>

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