

DL-Alanine, N-methyl-N-(but-3-yn-1-yloxy carbonyl)-, but-3-yn-1-yl ester

Inchi: CN(C)C(=O)OCC#C
InchiKey: AWJWXPXAWCNVRX-UHFFFAOYSA-N

Formula: C13H17NO4

SMILES: C#CCCOC(=O)C(C)N(C)C(=O)OCCC#C

Mol. weight [g/mol]: 251.28

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 145.22 | kJ/mol | Joback Method |
| hf | -155.20 | kJ/mol | Joback Method |
| hfus | 40.45 | kJ/mol | Joback Method |
| hvap | 64.22 | kJ/mol | Joback Method |
| log10ws | -2.24 | | Crippen Method |
| logp | 1.033 | | Crippen Method |
| mvol | 201.690 | ml/mol | McGowan Method |
| pc | 2329.27 | kPa | Joback Method |
| rinpol | 1684.00 | | NIST Webbook |
| rinpol | 1684.00 | | NIST Webbook |
| tb | 641.66 | K | Joback Method |
| tc | 838.17 | K | Joback Method |
| tf | 492.00 | K | Joback Method |
| vc | 0.748 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 517.38 | J/molxK | 641.66 | Joback Method |
| cpg | 530.97 | J/molxK | 674.41 | Joback Method |
| cpg | 543.81 | J/molxK | 707.16 | Joback Method |
| cpg | 555.92 | J/molxK | 739.91 | Joback Method |
| cpg | 567.31 | J/molxK | 772.67 | Joback Method |
| cpg | 578.01 | J/molxK | 805.42 | Joback Method |
| cpg | 588.03 | J/molxK | 838.17 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U392713&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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

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

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