

dl-c-Allylglycine

| | |
|-----------------------------|--|
| Other names: | dl-2-Amino-1-pentenoic acid 4-Pentenoic acid, 2-amino-, (.+/-.)- 2-Amino-4-pentenoic acid DL-2-aminopent-4-enoic acid |
| Inchi: | InChI=1S/C5H9NO2/c1-2-3-4(6)5(7)8/h2,4H,1,3,6H2,(H,7,8) |
| InchiKey: | WNNNWFKQCKFSDK-UHFFFAOYSA-N |
| Formula: | C5H9NO2 |
| SMILES: | C=CCC(N)C(=O)O |
| Mol. weight [g/mol]: | 115.13 |
| CAS: | 7685-44-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -122.67 | kJ/mol | Joback Method |
| hf | -257.40 | kJ/mol | Joback Method |
| hfus | 14.79 | kJ/mol | Joback Method |
| hvap | 59.73 | kJ/mol | Joback Method |
| log10ws | -0.41 | | Crippen Method |
| logp | -0.026 | | Crippen Method |
| mcvol | 94.430 | ml/mol | McGowan Method |
| pc | 4849.43 | kPa | Joback Method |
| tb | 528.62 | K | Joback Method |
| tc | 719.54 | K | Joback Method |
| tf | 323.36 | K | Joback Method |
| vc | 0.344 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 213.68 | J/molxK | 528.62 | Joback Method |
| cpg | 221.39 | J/molxK | 560.44 | Joback Method |
| cpg | 228.69 | J/molxK | 592.26 | Joback Method |
| cpg | 235.61 | J/molxK | 624.08 | Joback Method |
| cpg | 242.15 | J/molxK | 655.90 | Joback Method |

| | | | | |
|-----|--------|---------|--------|---------------|
| cpg | 248.33 | J/mol×K | 687.72 | Joback Method |
| cpg | 254.16 | J/mol×K | 719.54 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=C7685441&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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 |

Latest version available from:

<https://www.chemeo.com/cid/96-716-1/dl-c-Allylglycine.pdf>

Generated by Cheméo on 2024-04-29 18:21:53.860677596 +0000 UTC m=+16704162.781254970.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.