

Aspartic acid, N-acetyl-, diethyl ester, L-

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|----------------------|---|
| Other names: | (I) N-acetylaspartic acid, diethyl ester |
| Inchi: | InChI=1S/C10H17NO5/c1-4-15-9(13)6-8(11-7(3)12)10(14)16-5-2/h8H,4-6H2,1-3H3,(H,11) |
| InchiKey: | XQGDGRNHLJLQOV-UHFFFAOYSA-N |
| Formula: | C10H17NO5 |
| SMILES: | CCOC(=O)CC(N=C(C(O)C(=O)OCC)C(=O)OCC |
| Mol. weight [g/mol]: | 231.25 |
| CAS: | 1069-39-2 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | -824.41 | kJ/mol | Joback Method |
| hvap | 75.85 | kJ/mol | Joback Method |
| log10ws | -0.83 | | Crippen Method |
| logp | 0.848 | | Crippen Method |
| mcvol | 178.190 | ml/mol | McGowan Method |
| pc | 2298.11 | kPa | Joback Method |
| tb | 749.08 | K | Joback Method |
| tc | 941.73 | K | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-------|--------|-----------------|--------------|
| hvapt | 76.00 | kJ/mol | 463.00 | NIST Webbook |

Sources

| | |
|-----------------|---|
| 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 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1069392&Units=SI |

Legend

| | |
|-----------------|---|
| hf: | Enthalpy of formation at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |
| hvapt: | Enthalpy of vaporization at a given temperature |
| 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 |

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