

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

Inchi: InChI=1S/C24H45NO4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-28-23(26)19-20-2
InchiKey: AUHLJGCYYCNHOC-UHFFFAOYSA-N
Formula: C24H45NO4
SMILES: C=CCOC(O)=NCCC(=O)OCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 411.62

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | -870.08 | kJ/mol | Joback Method |
| hvap | 99.99 | kJ/mol | Joback Method |
| log10ws | -7.15 | | Crippen Method |
| logp | 6.908 | | Crippen Method |
| mcvol | 369.580 | ml/mol | McGowan Method |
| pc | 835.79 | kPa | Joback Method |
| rinpol | 3059.00 | | NIST Webbook |
| rinpol | 3059.00 | | NIST Webbook |
| tb | 1012.65 | K | Joback Method |
| tc | 1254.46 | K | Joback Method |

Sources

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=U321044&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

hf: Enthalpy of formation 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 |

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