

D-Alanine, N-allyloxycarbonyl-, tetradecyl ester

Inchi: InChI=1S/C21H39NO4/c1-4-6-7-8-9-10-11-12-13-14-15-16-18-25-20(23)19(3)22-21(24)2
InchiKey: VHDLCLCNKTWES-UHFFFAOYSA-N
Formula: C21H39NO4
SMILES: C=CCOC(O)=NC(C)C(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 369.54

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | -813.44 | kJ/mol | Joback Method |
| hvap | 92.92 | kJ/mol | Joback Method |
| log10ws | -6.01 | | Crippen Method |
| logp | 5.736 | | Crippen Method |
| mcvol | 327.310 | ml/mol | McGowan Method |
| pc | 999.54 | kPa | Joback Method |
| rinpol | 2514.00 | | NIST Webbook |
| rinpol | 2514.00 | | NIST Webbook |
| tb | 943.57 | K | Joback Method |
| tc | 1156.81 | K | Joback Method |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=U347737&Units=SI>

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 |
| rinpola: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |

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