

«beta»-Alanine, N-acryloyl-, hexadecyl ester

Inchi: InChI=1S/C22H41NO3/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-20-26-22(25)18-19-23-2
InchiKey: WIOZKABCIJIXOA-UHFFFAOYSA-N
Formula: C22H41NO3
SMILES: C=CC(O)=NCCC(=O)OCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 367.57

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | -696.58 | kJ/mol | Joback Method |
| hvap | 93.12 | kJ/mol | Joback Method |
| log10ws | -6.73 | | Crippen Method |
| logp | 6.543 | | Crippen Method |
| mcvol | 335.530 | ml/mol | McGowan Method |
| pc | 946.75 | kPa | Joback Method |
| rinpol | 2825.00 | | NIST Webbook |
| rinpol | 2825.00 | | NIST Webbook |
| tb | 944.47 | K | Joback Method |
| tc | 1158.94 | K | Joback Method |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321685&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

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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