

«beta»-Alanine, N-caproyl-, tetradecyl ester

Inchi: InChI=1S/C23H45NO3/c1-3-5-7-8-9-10-11-12-13-14-15-17-21-27-23(26)19-20-24-22(25)
InchiKey: VDBNJRPKDOGMMI-UHFFFAOYSA-N
Formula: C23H45NO3
SMILES: CCCCCCCCCCCCCOC(=O)CCN=C(O)CCCCC
Mol. weight [g/mol]: 383.61

Physical Properties

Property code	Value	Unit	Source
hf	-842.65	kJ/mol	Joback Method
hvap	96.02	kJ/mol	Joback Method
log10ws	-7.30		Crippen Method
logp	7.158		Crippen Method
mcvol	353.920	ml/mol	McGowan Method
pc	871.19	kPa	Joback Method
rinpol	2933.00		NIST Webbook
rinpol	2933.00		NIST Webbook
tb	970.67	K	Joback Method
tc	1195.73	K	Joback Method

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=U321789&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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