«beta»-Alanine, N-cyclohexylcarbonyl-, octyl ester

Inchi: InChI=1S/C18H33NO3/c1-2-3-4-5-6-10-15-22-17(20)13-14-19-18(21)16-11-8-7-9-12-16/h
InchiKey: ZNEXMEKDBPMBRM-UHFFFAOYSA-N
Formula: C18H33NO3
SMILES: CCCCCCCCOC(=O)CCN=C(O)C1CCCCC1
Mol. weight [g/mol]: 311.46

Physical Properties

Property code	Value	Unit	Source
hf	-685.13	kJ/mol	Joback Method
hvap	85.32	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	4.817		Crippen Method
mcvol	272.610	ml/mol	McGowan Method
pc	1368.70	kPa	Joback Method
rinpol	2457.00		NIST Webbook
rinpol	2457.00		NIST Webbook
tb	875.82	K	Joback Method
tc	1078.72	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321965&Units=SI
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

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