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

Inchi: InChI=1S/C18H35NO3/c1-3-5-7-8-9-10-12-16-22-18(21)14-15-19-17(20)13-11-6-4-2/h3-1
InchiKey: WBHNVWZAOOOOFY-UHFFFAOYSA-N
Formula: C18H35NO3
SMILES: CCCCCCCCCOC(=O)CCN=C(O)CCCCC
Mol. weight [g/mol]: 313.48

Physical Properties

Property code	Value	Unit	Source
hf	-739.45	kJ/mol	Joback Method
hvap	84.89	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	5.207		Crippen Method
mcvol	283.470	ml/mol	McGowan Method
pc	1182.53	kPa	Joback Method
rinpol	2374.00		NIST Webbook
rinpol	2374.00		NIST Webbook
tb	856.27	K	Joback Method
tc	1049.03	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321786&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