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

Inchi: InChI=1S/C20H39NO3/c1-3-5-7-9-10-12-14-18-24-20(23)16-17-21-19(22)15-13-11-8-6-4
InchiKey: JKHDYLJCIZHMEW-UHFFFAOYSA-N
Formula: C20H39NO3
SMILES: CCCCCCCCCOC(=O)CCN=C(O)CCCCCCC
Mol. weight [g/mol]: 341.53

Physical Properties

Property code	Value	Unit	Source
hf	-780.73	kJ/mol	Joback Method
hvap	89.34	kJ/mol	Joback Method
log10ws	-6.04		Crippen Method
logp	5.987		Crippen Method
mcvol	311.650	ml/mol	McGowan Method
pc	1040.58	kPa	Joback Method
rinpol	2579.00		NIST Webbook
rinpol	2579.00		NIST Webbook
tb	902.03	K	Joback Method
tc	1104.61	K	Joback Method

Sources

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=U321815&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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