

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

Inchi: InChI=1S/C19H37NO3/c1-3-5-7-9-11-13-17-23-19(22)15-16-20-18(21)14-12-10-8-6-4-2/
InchiKey: DAJDGOYHLCLAAJ-UHFFFAOYSA-N
Formula: C19H37NO3
SMILES: CCCCCCCCOC(=O)CCN=C(O)CCCCCCC
Mol. weight [g/mol]: 327.50

Physical Properties

Property code	Value	Unit	Source
hf	-760.09	kJ/mol	Joback Method
hvap	87.12	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	5.597		Crippen Method
mcvol	297.560	ml/mol	McGowan Method
pc	1108.15	kPa	Joback Method
rinpol	2483.00		NIST Webbook
rinpol	2483.00		NIST Webbook
tb	879.15	K	Joback Method
tc	1076.36	K	Joback Method

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321814&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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