

L-Norvaline, N-octyloxycarbonyl-, pentyl ester

Inchi: InChI=1S/C19H37NO4/c1-4-7-9-10-11-13-16-24-19(22)20-17(14-6-3)18(21)23-15-12-8-5
InchiKey: ZMFKAUUXODKXAR-QGZVFWFLSA-N
Formula: C19H37NO4
SMILES: CCCCCCOC(O)=NC(CCC)C(=O)OCCCCC
Mol. weight [g/mol]: 343.50

Physical Properties

Property code	Value	Unit	Source
hf	-897.59	kJ/mol	Joback Method
hvap	89.14	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	5.180		Crippen Method
mcvol	303.430	ml/mol	McGowan Method
pc	1101.54	kPa	Joback Method
rinpol	2291.00		NIST Webbook
rinpol	2291.00		NIST Webbook
tb	901.13	K	Joback Method
tc	1103.27	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U392845&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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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