

L-Norvaline, N-decyloxycarbonyl-, undecyl ester

Inchi: InChI=1S/C27H53NO4/c1-4-7-9-11-13-15-17-18-20-23-31-26(29)25(22-6-3)28-27(30)32-3
InchiKey: RZXVQMDUOBZVLS-RUZDIDTESA-N
Formula: C27H53NO4
SMILES: CCCCCCCCCCOC(=O)C(CCC)N=C(O)CCCCCCCCC
Mol. weight [g/mol]: 455.71

Physical Properties

Property code	Value	Unit	Source
hf	-1062.71	kJ/mol	Joback Method
hvap	106.95	kJ/mol	Joback Method
log10ws	-8.66		Crippen Method
logp	8.300		Crippen Method
mcvol	416.150	ml/mol	McGowan Method
pc	699.50	kPa	Joback Method
rinpol	3076.00		NIST Webbook
rinpol	3076.00		NIST Webbook
tb	1084.17	K	Joback Method
tc	1368.09	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U392855&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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