

L-Norvaline, N-((1R)-(-)-menthyloxycarbonyl)-, undecyl ester

Inchi: InChI=1S/C27H51NO4/c1-6-8-9-10-11-12-13-14-15-19-31-26(29)24(16-7-2)28-27(30)32-31
InchiKey: WJWAZCKIUWOFRG-UHFFFAOYSA-N
Formula: C27H51NO4
SMILES: CCCCCCCCCCOC(=O)C(CCC)N=C(O)OC1CC(C)CCC1C(C)C
Mol. weight [g/mol]: 453.70

Physical Properties

Property code	Value	Unit	Source
hf	-1054.35	kJ/mol	Joback Method
hvap	106.37	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	7.621		Crippen Method
mcvol	405.290	ml/mol	McGowan Method
pc	757.23	kPa	Joback Method
rinpol	2956.00		NIST Webbook
rinpol	2956.00		NIST Webbook
tb	1093.94	K	Joback Method
tc	1354.93	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U392884&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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