

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

Inchi:	InChI=1S/C28H53NO4/c1-6-8-9-10-11-12-13-14-15-16-20-32-27(30)25(17-7-2)29-28(31)
InchiKey:	LCIQVNUQTAWYEC-UHFFFAOYSA-N
Formula:	C28H53NO4
SMILES:	CCCCCCCCCCCCOC(=O)C(CCC)N=C(O)OC1CC(C)CCC1C(C)C
Mol. weight [g/mol]:	467.72

Physical Properties

Property code	Value	Unit	Source
hf	-1074.99	kJ/mol	Joback Method
hvap	108.60	kJ/mol	Joback Method
log10ws	-8.36		Crippen Method
logp	8.011		Crippen Method
mcvol	419.380	ml/mol	McGowan Method
pc	718.76	kPa	Joback Method
rinpol	3055.00		NIST Webbook
rinpol	3055.00		NIST Webbook
tb	1116.82	K	Joback Method
tc	1390.20	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=U392885&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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