

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

Inchi: InChI=1S/C19H35NO4/c1-6-8-16(18(21)23-11-7-2)20-19(22)24-17-12-14(5)9-10-15(17)1
InchiKey: YQTMKBAOXJDYGX-UHFFFAOYSA-N
Formula: C19H35NO4
SMILES: CCCOC(=O)C(CCC)N=C(O)OC1CC(C)CCC1C(C)C
Mol. weight [g/mol]: 341.49

Physical Properties

Property code	Value	Unit	Source
hf	-889.23	kJ/mol	Joback Method
hvap	88.56	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.500		Crippen Method
mcvol	292.570	ml/mol	McGowan Method
pc	1217.44	kPa	Joback Method
rinpol	2172.00		NIST Webbook
rinpol	2172.00		NIST Webbook
tb	910.90	K	Joback Method
tc	1119.21	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U392877&Units=SI>
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>

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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