

L-Valine, N-(3-cyclopentylpropionyl)-, isohexyl ester

Inchi:	InChI=1S/C19H35NO3/c1-14(2)8-7-13-23-19(22)18(15(3)4)20-17(21)12-11-16-9-5-6-10-
InchiKey:	OLTOEUUYUDQEXLC-UHFFFAOYSA-N
Formula:	C19H35NO3
SMILES:	CC(C)CCCOC(=O)C(N=C(O)CCC1CCCC1)C(C)C
Mol. weight [g/mol]:	325.49

Physical Properties

Property code	Value	Unit	Source
hf	-715.45	kJ/mol	Joback Method
hvap	86.21	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.917		Crippen Method
mcvol	286.700	ml/mol	McGowan Method
pc	1275.51	kPa	Joback Method
rinpol	2280.00		NIST Webbook
rinpol	2280.00		NIST Webbook
tb	893.11	K	Joback Method
tc	1098.95	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=U346657&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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