

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

Inchi:	InChI=1S/C28H53NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-18-23-32-28(31)27(24(2)3)29-
InchiKey:	ZHKWADHADPDQHW-UHFFFAOYSA-N
Formula:	C28H53NO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(N=C(O)CCC1CCCC1)C(C)C
Mol. weight [g/mol]:	451.73

Physical Properties

Property code	Value	Unit	Source
hf	-895.93	kJ/mol	Joback Method
hvap	106.63	kJ/mol	Joback Method
log10ws	-8.91		Crippen Method
logp	8.572		Crippen Method
mcvol	413.510	ml/mol	McGowan Method
pc	741.64	kPa	Joback Method
rinpol	3292.00		NIST Webbook
rinpol	3292.00		NIST Webbook
tb	1099.47	K	Joback Method
tc	1367.55	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=U346661&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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