

L-Valine, N-(3-methylbenzoyl)-, tetradecyl ester

Inchi:	InChI=1S/C27H45NO3/c1-5-6-7-8-9-10-11-12-13-14-15-16-20-31-27(30)25(22(2)3)28-26
InchiKey:	SNOSUXTZZNPDFJ-UHFFFAOYSA-N
Formula:	C27H45NO3
SMILES:	CCCCCCCCCCCCCOC(=O)C(N=C(O)c1cccc(C)c1)C(C)C
Mol. weight [g/mol]:	431.65

Physical Properties

Property code	Value	Unit	Source
hf	-710.71	kJ/mol	Joback Method
hvap	107.09	kJ/mol	Joback Method
log10ws	-8.10		Crippen Method
logp	7.569		Crippen Method
mcvol	386.520	ml/mol	McGowan Method
pc	845.05	kPa	Joback Method
rinpol	3198.00		NIST Webbook
rinpol	3198.00		NIST Webbook
tb	1092.97	K	Joback Method
tc	1348.64	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=U346652&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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