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

Inchi: InChI=1S/C24H39NO3/c1-5-6-7-8-9-10-11-12-13-17-28-24(27)22(19(2)3)25-23(26)21-16
InchiKey: WWLJAFJYLUAJTR-UHFFFAOYSA-N
Formula: C24H39NO3
SMILES: CCCCCCCCCCCOC(=O)C(N=C(O)c1cccc(C)c1)C(C)C
Mol. weight [g/mol]: 389.57

Physical Properties

Property code	Value	Unit	Source
hf	-648.79	kJ/mol	Joback Method
hvap	100.41	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	6.398		Crippen Method
mcvol	344.250	ml/mol	McGowan Method
pc	1006.53	kPa	Joback Method
rinpol	2875.00		NIST Webbook
rinpol	2875.00		NIST Webbook
tb	1024.33	K	Joback Method
tc	1254.89	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346650&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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