

L-Valine, N-(2-methoxybenzoyl)-, undecyl ester

Inchi: InChI=1S/C24H39NO4/c1-5-6-7-8-9-10-11-12-15-18-29-24(27)22(19(2)3)25-23(26)20-16
InchiKey: TXYWWXUVVMJYAL-UHFFFAOYSA-N
Formula: C24H39NO4
SMILES: CCCCCCCCCCOC(=O)C(N=C(O)c1ccccc1OC)C(C)C
Mol. weight [g/mol]: 405.57

Physical Properties

Property code	Value	Unit	Source
hf	-781.01	kJ/mol	Joback Method
hvap	102.82	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	6.098		Crippen Method
mcvol	350.120	ml/mol	McGowan Method
pc	995.76	kPa	Joback Method
rinpol	3014.00		NIST Webbook
rinpol	3014.00		NIST Webbook
tb	1046.75	K	Joback Method
tc	1284.03	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346596&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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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