

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

Inchi:	InChI=1S/C22H35NO4/c1-5-6-7-8-9-10-13-16-27-22(25)20(17(2)3)23-21(24)18-14-11-12
InchiKey:	WVCPPOWOQBXIKD-UHFFFAOYSA-N
Formula:	C22H35NO4
SMILES:	CCCCCCCCCOC(=O)C(N=C(O)c1ccccc1OC)C(C)C
Mol. weight [g/mol]:	377.52

Physical Properties

Property code	Value	Unit	Source
hf	-739.73	kJ/mol	Joback Method
hvap	98.37	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.318		Crippen Method
mcvol	321.940	ml/mol	McGowan Method
pc	1128.35	kPa	Joback Method
rinpol	2793.00		NIST Webbook
rinpol	2793.00		NIST Webbook
tb	1000.99	K	Joback Method
tc	1225.50	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=U346594&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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