

L-Valine, N-dimethylaminomethylene-, butyl ester

Inchi: InChI=1S/C12H24N2O2/c1-6-7-8-16-12(15)11(10(2)3)13-9-14(4)5/h9-11H,6-8H2,1-5H3
InchiKey: CIQLNMPTUROYST-UHFFFAOYSA-N
Formula: C12H24N2O2
SMILES: CCCCOC(=O)C(N=CN(C)C)C(C)C
Mol. weight [g/mol]: 228.33

Physical Properties

Property code	Value	Unit	Source
hf	-396.62	kJ/mol	Joback Method
hvap	56.04	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	1.944		Crippen Method
mcvol	203.040	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	1513.00		NIST Webbook
rinpol	1513.00		NIST Webbook
tb	638.49	K	Joback Method
tc	827.39	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375637&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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