

L-Isoleucine, N-dimethylaminomethylene-, butyl ester

Inchi: InChI=1S/C13H26N2O2/c1-6-8-9-17-13(16)12(11(3)7-2)14-10-15(4)5/h10-12H,6-9H2,1-5
InchiKey: AQIGFQBULJUEKA-UHFFFAOYSA-N
Formula: C13H26N2O2
SMILES: CCCCOC(=O)C(N=CN(C)C)C(C)CC
Mol. weight [g/mol]: 242.36

Physical Properties

Property code	Value	Unit	Source
hf	-417.26	kJ/mol	Joback Method
hvap	58.27	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	2.334		Crippen Method
mcvol	217.130	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	1602.00		NIST Webbook
tb	661.37	K	Joback Method
tc	848.60	K	Joback Method

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375631&Units=SI>

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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