

L-Isoleucine, N-dimethylaminomethylene-, ethyl ester

Inchi:	InChI=1S/C11H22N2O2/c1-6-9(3)10(11(14)15-7-2)12-8-13(4)5/h8-10H,6-7H2,1-5H3
InchiKey:	FYQLEJWDNZYUQT-UHFFFAOYSA-N
Formula:	C11H22N2O2
SMILES:	CCOC(=O)C(N=CN(C)C)C(C)CC
Mol. weight [g/mol]:	214.30

Physical Properties

Property code	Value	Unit	Source
hf	-375.98	kJ/mol	Joback Method
hvap	53.82	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	1.554		Crippen Method
mcvol	188.950	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
rinpol	1427.00		NIST Webbook
rinpol	1427.00		NIST Webbook
tb	615.61	K	Joback Method
tc	806.50	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375632&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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