L-Isoleucine, N-dimethylaminomethylene-

Inchi: InChI=1S/C9H18N2O2/c1-5-7(2)8(9(12)13)10-6-11(3)4/h6-8H,5H2,1-4H3,(H,12,13)
InchiKey: GITMYGXRNIABBQ-UHFFFAOYSA-N
Formula: C9H18N2O2
SMILES: CCC(C)C(N=CN(C)C)C(=O)O
Mol. weight [g/mol]: 186.25

Physical Properties

Property code	Value	Unit	Source
hf	-354.71	kJ/mol	Joback Method
hvap	63.63	kJ/mol	Joback Method
log10ws	-0.79		Crippen Method
logp	1.076		Crippen Method
mcvol	160.770	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
rinpol	1578.00		NIST Webbook
tb	639.61	K	Joback Method
tc	826.42	K	Joback Method

Sources

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=U375630&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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