L-Isoleucine, N-dimethylaminomethylene-, methyl ester

Inchi: InChI=1S/C10H20N2O2/c1-6-8(2)9(10(13)14-5)11-7-12(3)4/h7-9H,6H2,1-5H3
InchiKey: AQZUPSFYTJWYPE-UHFFFAOYSA-N
Formula: C10H20N2O2
SMILES: CCC(C)C(N=CN(C)C)C(=O)OC
Mol. weight [g/mol]: 200.28

Physical Properties

Property code	Value	Unit	Source
hf	-355.34	kJ/mol	Joback Method
hvap	51.59	kJ/mol	Joback Method
log10ws	-0.97		Crippen Method
logp	1.164		Crippen Method
mcvol	174.860	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
rinpol	1374.00		NIST Webbook
rinpol	1374.00		NIST Webbook
tb	592.73	K	Joback Method
tc	785.90	K	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U375633&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