L-Leucine, N-dimethylaminomethylene-, methyl ester

Inchi: InChI=1S/C10H20N2O2/c1-8(2)6-9(10(13)14-5)11-7-12(3)4/h7-9H,6H2,1-5H3

InchiKey: JOLYLOZRGAOJJW-UHFFFAOYSA-N

Formula: C10H20N2O2

SMILES: COC(=O)C(CC(C)C)N=CN(C)C

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	1373.00		NIST Webbook
tb	592.73	K	Joback Method
tc	785.90	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=U375626&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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