L-Valine, N-dimethylaminomethylene-, methyl ester

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

Physical Properties

Property code	Value	Unit	Source
hf	-334.70	kJ/mol	Joback Method
hvap	49.36	kJ/mol	Joback Method
log10ws	-0.55		Crippen Method
logp	0.774		Crippen Method
mcvol	160.770	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
rinpol	1282.00		NIST Webbook
tb	569.85	K	Joback Method
tc	765.52	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375639&Units=SI
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

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