L-Alanine, N-dimethylaminomethylene-, methyl ester

Inchi: InChI=1S/C7H14N2O2/c1-6(7(10)11-4)8-5-9(2)3/h5-6H,1-4H3
InchiKey: NXWQXTNKKBBUNZ-UHFFFAOYSA-N
Formula: C7H14N2O2
SMILES: COC(=O)C(C)N=CN(C)C
Mol. weight [g/mol]: 158.20

Physical Properties

Property code	Value	Unit	Source
hf	-288.14	kJ/mol	Joback Method
hvap	45.30	kJ/mol	Joback Method
log10ws	0.04		Crippen Method
logp	0.138		Crippen Method
mcvol	132.590	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method
rinpol	1173.00		NIST Webbook
rinpol	1173.00		NIST Webbook
tb	524.53	K	Joback Method
tc	721.45	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375642&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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