3-Aminobutanoic acid, N-dimethylaminomethylene-, methyl ester

Inchi: InChI=1S/C8H16N2O2/c1-7(5-8(11)12-4)9-6-10(2)3/h6-7H,5H2,1-4H3
InchiKey: QJWFAOFRLGFBRZ-UHFFFAOYSA-N
Formula: C8H16N2O2
SMILES: COC(=O)CC(C)N=CN(C)C
Mol. weight [g/mol]: 172.22

Physical Properties

Property code	Value	Unit	Source
hf	-308.78	kJ/mol	Joback Method
hvap	47.53	kJ/mol	Joback Method
log10ws	-0.38		Crippen Method
logp	0.528		Crippen Method
mcvol	146.680	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
rinpol	1193.00		NIST Webbook
rinpol	1193.00		NIST Webbook
tb	547.41	K	Joback Method
tc	741.73	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=U375776&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