O-Methyl-DL-serine, N-dimethylaminomethylene-, methyl ester

Inchi: InChI=1S/C8H16N2O3/c1-10(2)6-9-7(5-12-3)8(11)13-4/h6-7H,5H2,1-4H3
InchiKey: HPRPLWMMVVDNMT-UHFFFAOYSA-N
Formula: C8H16N2O3
SMILES: COCC(N=CN(C)C)C(=O)OC
Mol. weight [g/mol]: 188.22

Physical Properties

Property code	Value	Unit	Source
hf	-441.00	kJ/mol	Joback Method
hvap	49.94	kJ/mol	Joback Method
log10ws	0.54		Crippen Method
logp	-0.236		Crippen Method
mcvol	152.550	ml/mol	McGowan Method
pc	2365.67	kPa	Joback Method
rinpol	1354.00		NIST Webbook
rinpol	1354.00		NIST Webbook
tb	569.83	K	Joback Method
tc	762.66	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=U375997&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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