1-Aminocyclopropanecarboxylic acid, N-dimethylaminomethylene-, methyl ester

Inchi: InChI=1S/C8H14N2O2/c1-10(2)6-9-8(4-5-8)7(11)12-3/h6H,4-5H2,1-3H3
InchiKey: UZEDWUMCEZKWKE-UHFFFAOYSA-N
Formula: C8H14N2O2
SMILES: COC(=O)C1(N=CN(C)C)CC1
Mol. weight [g/mol]: 170.21

Physical Properties

Property code	Value	Unit	Source
hf	-215.46	kJ/mol	Joback Method
hvap	46.68	kJ/mol	Joback Method
log10ws	-0.27		Crippen Method
logp	0.282		Crippen Method
mcvol	135.820	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	1300.00		NIST Webbook
rinpol	1300.00		NIST Webbook
tb	554.83	K	Joback Method
tc	767.15	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=U375510&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