L-Aspartic acid, N-dimethylaminomethylene-, dimethyl ester

Inchi: InChI=1S/C9H16N2O4/c1-11(2)6-10-7(9(13)15-4)5-8(12)14-3/h6-7H,5H2,1-4H3
InchiKey: DIDALCHIHXQMBM-UHFFFAOYSA-N
Formula: C9H16N2O4
SMILES: COC(=O)CC(N=CN(C)C)C(=O)OC
Mol. weight [g/mol]: 216.23

Physical Properties

Property code	Value	Unit	Source
hf	-574.22	kJ/mol	Joback Method
hvap	58.91	kJ/mol	Joback Method
log10ws	0.34		Crippen Method
logp	-0.319		Crippen Method
mcvol	168.210	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinpol	1508.00		NIST Webbook
rinpol	1508.00		NIST Webbook
tb	646.58	K	Joback Method
tc	844.35	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375643&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