S-Carboxymethyl-L-cysteine, N-dimethylaminomethylene, diethyl ester

Inchi: InChI=1S/C12H22N2O4S/c1-5-17-11(15)8-19-7-10(12(16)18-6-2)13-9-14(3)4/h9-10H,5-8

InchiKey: KIMLQTYYXYYATQ-UHFFFAOYSA-N

Formula: C12H22N2O4S

SMILES: CCOC(=O)CSCC(N=CN(C)C)C(=O)OCC

Mol. weight [g/mol]: 290.38

Physical Properties

Property code	Value	Unit	Source
hf	-594.27	kJ/mol	Joback Method
hvap	72.40	kJ/mol	Joback Method
log10ws	-0.80		Crippen Method
logp	0.804		Crippen Method
mcvol	226.830	ml/mol	McGowan Method
pc	1795.46	kPa	Joback Method
rinpol	1993.00		NIST Webbook
rinpol	1993.00		NIST Webbook
tb	784.00	K	Joback Method
tc	989.82	K	Joback Method

Sources

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=U376186&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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