S-carbethoxymethyl-L-cysteine, N-dimethylaminomethylene-, dimethyl ester

Inchi: InChI=1S/C10H18N2O4S/c1-12(2)7-11-8(10(14)16-4)5-17-6-9(13)15-3/h7-8H,5-6H2,1-4

InchiKey: CYNRXKFNBAPCMP-UHFFFAOYSA-N

Formula: C10H18N2O4S

SMILES: COC(=O)CSCC(N=CN(C)C)C(=O)OC

Mol. weight [g/mol]: 262.33

Physical Properties

Property code	Value	Unit	Source
hf	-552.99	kJ/mol	Joback Method
hvap	67.95	kJ/mol	Joback Method
log10ws	0.04		Crippen Method
logp	0.024		Crippen Method
mcvol	198.650	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	1882.00		NIST Webbook
tb	738.24	K	Joback Method
tc	947.99	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=U376187&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