L-Cystathionine, N,N'-bis(dimethylaminomethylene)-, dimethyl ester

Inchi: InChI=1S/C15H28N4O4S/c1-18(2)10-16-12(14(20)22-5)7-8-24-9-13(15(21)23-6)17-11-19

InchiKey: QFHHZCXRDCKSIP-UHFFFAOYSA-N

Formula: C15H28N4O4S

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

Mol. weight [g/mol]: 360.47

Physical Properties

Property code	Value	Unit	Source
hf	-511.72	kJ/mol	Joback Method
hvap	84.05	kJ/mol	Joback Method
log10ws	-0.39		Crippen Method
logp	0.373		Crippen Method
mcvol	284.760	ml/mol	McGowan Method
pc	1325.20	kPa	Joback Method
rinpol	2559.00		NIST Webbook
tb	941.32	K	Joback Method
tc	1160.71	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375994&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