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

Inchi: InChI=1S/C17H32N4O4S/c1-7-24-16(22)14(18-12-20(3)4)9-10-26-11-15(17(23)25-8-2)19

InchiKey: NCBAWTFQLBEJKQ-UHFFFAOYSA-N

Formula: C17H32N4O4S

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

Mol. weight [g/mol]: 388.52

Physical Properties

Property code	Value	Unit	Source
hf	-553.00	kJ/mol	Joback Method
hvap	88.50	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	1.153		Crippen Method
mcvol	312.940	ml/mol	McGowan Method
pc	1157.71	kPa	Joback Method
rinpol	2645.00		NIST Webbook
tb	987.08	K	Joback Method
tc	1210.66	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375993&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