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

Inchi: InChI=1S/C16H30N4O4S2/c1-19(2)11-17-13(15(21)23-5)7-9-25-26-10-8-14(16(22)24-6)18-12-20(3)4/h11-14H,7-10H2,1-6H3/b17-11+,18-12+

InchiKey: DFZPRTRNBDDJNU-UHFFFAOYSA-N

Formula: C16H30N4O4S2

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

Mol. weight [g/mol]: 406.56

Physical Properties

Property code	Value	Unit	Source
hf	-490.49	kJ/mol	Joback Method
hvap	93.09	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.411		Crippen Method
mcvol	315.200	ml/mol	McGowan Method
pc	1252.15	kPa	Joback Method
rinpol	2921.00		NIST Webbook
tb	1032.98	K	Joback Method
tc	1267.87	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=U375485&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