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

Inchi: InChI=1S/C18H34N4O4S2/c1-7-25-17(23)15(19-13-21(3)4)9-11-27-28-12-10-16(18(24)2
InchiKey: LIEFWTZUPFGZTD-UHFFFAOYSA-N
Formula: C18H34N4O4S2
SMILES: CCOC(=O)C(CCSSCCC(N=CN(C)C)C(=O)OCC)N=CN(C)C
Mol. weight [g/mol]: 434.62

Physical Properties

Property code	Value	Unit	Source
hf	-531.77	kJ/mol	Joback Method
hvap	97.55	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.191		Crippen Method
mcvol	343.380	ml/mol	McGowan Method
pc	1097.90	kPa	Joback Method
rinpol	3043.00		NIST Webbook
tb	1078.74	K	Joback Method
tc	1320.78	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=U375486&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