

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

Inchi:
ester

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

InchiKey:

QFHHCXRDCSIP-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	2558.00		NIST Webbook
tb	941.32	K	Joback Method
tc	1160.71	K	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U375732&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

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

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