N(2),N(6)-Bis(dimethylaminomethylene)lysine methyl ester

Other names: L-Lysine, N,N'-bis(dimethylaminomethylene)-, methyl ester

Methyl 6-[[(E)-(dimethylamino)methylidene]amino]-2-[[(Z)-(dimethylamino)methylidene]amino]he

Inchi: InChI=1S/C13H26N4O2/c1-16(2)10-14-9-7-6-8-12(13(18)19-5)15-11-17(3)4/h10-12H,6-9

InchiKey: VRYPGRZLBVMBCT-GFCCVEGCSA-N

Formula: C13H26N4O2

SMILES: COC(=O)C(CCCCN=CN(C)C)N=CN(C)C

Mol. weight [g/mol]: 270.37

CAS: 70102-41-9

Physical Properties

Property code	Value	Unit	Source
hf	-262.23	kJ/mol	Joback Method
hvap	64.01	kJ/mol	Joback Method
log10ws	-0.70		Crippen Method
logp	0.878		Crippen Method
mcvol	232.790	ml/mol	McGowan Method
pc	1450.14	kPa	Joback Method
rinpol	2003.00		NIST Webbook
rinpol	2003.00		NIST Webbook
tb	750.93	K	Joback Method
tc	947.06	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C70102419&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