N(2),N(6)-BIS(DIMETHYLAMINOMETHYLENE)LYS 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-LBPRGKRZSA-N

Formula: C13H26N4O2

SMILES: COC(=O)[C@H](CCCCN=CN(C)C)N=CN(C)C

Mol. weight [g/mol]: 270.38

Physical Properties

Property code	Value	Unit	Source
logp	0.878		Crippen Method
mcvol	232.790	ml/mol	McGowan Method
rinpol	2003.00		NIST Webbook
rinpol	2003.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices