L-Citrulline, N,N'-bis(dimethylaminomethylene)-, methyl ester

Othernames: l-Ornithine, N2-[(dimethylamino)methylene]-N5-[[(dimethylamino)methylene]amino]carbonyl]-, methyl ester

Inchi: InChI=1S/C13H25N5O3/c1-17(2)9-15-11(12(19)21-5)7-6-8-14-13(20)16-10-18(3)4/h9-11

InchiKey: ZLRCGUYJYWKIIV-UHFFFAOYSA-N

Formula: C13H25N5O3

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

Mol. weight [g/mol]: 299.37

CAS: 59824-38-3

Physical Properties

Property code	Value	Unit	Source
hf	-321.34	kJ/mol	Joback Method
hvap	77.20	kJ/mol	Joback Method
log10ws	-0.64		Crippen Method
logp	0.198		Crippen Method
mcvol	244.340	ml/mol	McGowan Method
pc	1537.87	kPa	Joback Method
rinpol	2587.00		NIST Webbook
rinpol	2587.00		NIST Webbook
tb	854.97	K	Joback Method
tc	1061.32	K	Joback Method

Sources

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=C59824383&Units=SI

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

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

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