D-Ornithine, N,N'-bis(dimethylaminomethylene)-, methyl ester

Inchi: InChI=1S/C12H24N4O2/c1-15(2)9-13-8-6-7-11(12(17)18-5)14-10-16(3)4/h9-11H,6-8H2,1

InchiKey: ASPXRROIPAMVOV-UHFFFAOYSA-N

Formula: C12H24N4O2

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

Mol. weight [g/mol]: 256.34

Physical Properties

Property code	Value	Unit	Source
hf	-241.59	kJ/mol	Joback Method
hvap	61.79	kJ/mol	Joback Method
log10ws	-0.28		Crippen Method
logp	0.488		Crippen Method
mcvol	218.700	ml/mol	McGowan Method
pc	1562.28	kPa	Joback Method
rinpol	1906.00		NIST Webbook
tb	728.05	K	Joback Method
tc	925.44	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375799&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

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