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

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

InchiKey: MVIPRXQAGUIRBX-UHFFFAOYSA-N

Formula: C13H26N4O2

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

Mol. weight [g/mol]: 270.37

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	1956.00		NIST Webbook
rinpol	1956.00		NIST Webbook
tb	750.93	K	Joback Method
tc	947.06	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=U375798&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