DL-2-Aminoadipic acid, N-dimethylaminomethylene-, diethyl ester

Inchi: InChI=1S/C13H24N2O4/c1-5-18-12(16)9-7-8-11(13(17)19-6-2)14-10-15(3)4/h10-11H,5-9

InchiKey: FCYQAUJBCAEWAE-UHFFFAOYSA-N

Formula: C13H24N2O4

SMILES: CCOC(=O)CCCC(N=CN(C)C)C(=O)OCC

Mol. weight [g/mol]: 272.34

Physical Properties

Property code	Value	Unit	Source
hf	-656.78	kJ/mol	Joback Method
hvap	67.81	kJ/mol	Joback Method
log10ws	-1.33		Crippen Method
logp	1.241		Crippen Method
mcvol	224.570	ml/mol	McGowan Method
pc	1635.13	kPa	Joback Method
rinpol	1840.00		NIST Webbook
rinpol	1840.00		NIST Webbook
tb	738.10	K	Joback Method
tc	929.34	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375710&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