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

Inchi: InChI=1S/C11H20N2O4/c1-13(2)8-12-9(11(15)17-4)6-5-7-10(14)16-3/h8-9H,5-7H2,1-4H

InchiKey: BAIAPBRYYFVIEZ-UHFFFAOYSA-N

Formula: C11H20N2O4

SMILES: COC(=O)CCCC(N=CN(C)C)C(=O)OC

Mol. weight [g/mol]: 244.29

Physical Properties

Property code	Value	Unit	Source
hf	-615.50	kJ/mol	Joback Method
hvap	63.36	kJ/mol	Joback Method
log10ws	-0.49		Crippen Method
logp	0.461		Crippen Method
mcvol	196.390	ml/mol	McGowan Method
pc	1921.98	kPa	Joback Method
rinpol	1724.00		NIST Webbook
rinpol	1724.00		NIST Webbook
tb	692.34	K	Joback Method
tc	886.00	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375711&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

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