D-«alpha»-Cyclohexylglycine, N-dimethylaminomethylene-, ethyl ester

Inchi: InChI=1S/C13H24N2O2/c1-4-17-13(16)12(14-10-15(2)3)11-8-6-5-7-9-11/h10-12H,4-9H2

InchiKey: COCDVLHOTJURPC-UHFFFAOYSA-N

Formula: C13H24N2O2

SMILES: CCOC(=O)C(N=CN(C)C)C1CCCCC1

Mol. weight [g/mol]: 240.34

Physical Properties

Property code	Value	Unit	Source
hf	-357.66	kJ/mol	Joback Method
hvap	59.09	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	2.088		Crippen Method
mcvol	206.270	ml/mol	McGowan Method
pc	1867.55	kPa	Joback Method
rinpol	1712.00		NIST Webbook
rinpol	1712.00		NIST Webbook
tb	681.36	K	Joback Method
tc	893.35	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=U375806&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