

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

Inchi: InChI=1S/C12H22N2O2/c1-14(2)9-13-11(12(15)16-3)10-7-5-4-6-8-10/h9-11H,4-8H2,1-3H
InchiKey: QZUPLNAKZZMWNX-UHFFFAOYSA-N
Formula: C12H22N2O2
SMILES: COC(=O)C(N=CN(C)C)C1CCCCC1
Mol. weight [g/mol]: 226.32

Physical Properties

Property code	Value	Unit	Source
hf	-337.02	kJ/mol	Joback Method
hvap	56.86	kJ/mol	Joback Method
log10ws	-1.70		Crippen Method
logp	1.698		Crippen Method
mcvol	192.180	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpol	1661.00		NIST Webbook
tb	658.48	K	Joback Method
tc	873.83	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375807&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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