

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

Inchi: InChI=1S/C15H28N2O2/c1-4-5-11-19-15(18)14(16-12-17(2)3)13-9-7-6-8-10-13/h12-14H
InchiKey: LBTZBKQTKAJVPK-UHFFFAOYSA-N
Formula: C15H28N2O2
SMILES: CCCOC(=O)C(N=CN(C)C)C1CCCCC1
Mol. weight [g/mol]: 268.39

Physical Properties

Property code	Value	Unit	Source
hf	-398.94	kJ/mol	Joback Method
hvap	63.54	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.868		Crippen Method
mcvol	234.450	ml/mol	McGowan Method
pc	1592.35	kPa	Joback Method
rinpol	1891.00		NIST Webbook
rinpol	1891.00		NIST Webbook
tb	727.12	K	Joback Method
tc	933.57	K	Joback Method

Sources

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
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375805&Units=SI>

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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