3-Amino-3-(2-chlorophenyl)propionic acid, N-dimethylaminomethylene-, ethyl ester

Inchi: InChI=1S/C14H19ClN2O2/c1-4-19-14(18)9-13(16-10-17(2)3)11-7-5-6-8-12(11)15/h5-8,1

InchiKey: KPCDELOTIFFKIP-UHFFFAOYSA-N

Formula: C14H19ClN2O2

SMILES: CCOC(=O)CC(N=CN(C)C)c1ccccc1Cl

Mol. weight [g/mol]: 282.77

Physical Properties

Property code	Value	Unit	Source
hf	-223.30	kJ/mol	Joback Method
hvap	68.21	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.924		Crippen Method
mcvol	219.700	ml/mol	McGowan Method
pc	1832.54	kPa	Joback Method
rinpol	1961.00		NIST Webbook
rinpol	1961.00		NIST Webbook
tb	753.78	K	Joback Method
tc	972.38	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=U375832&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