

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

Inchi: InChI=1S/C13H17ClN2O2/c1-16(2)9-15-12(8-13(17)18-3)10-6-4-5-7-11(10)14/h4-7,9,12
InchiKey: MDOUGJZYOTUMSY-UHFFFAOYSA-N
Formula: C13H17ClN2O2
SMILES: COC(=O)CC(N=CN(C)C)c1ccccc1Cl
Mol. weight [g/mol]: 268.74

Physical Properties

Property code	Value	Unit	Source
hf	-202.66	kJ/mol	Joback Method
hvap	65.98	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.534		Crippen Method
mcvol	205.610	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
rinpol	1892.00		NIST Webbook
rinpol	1892.00		NIST Webbook
tb	730.90	K	Joback Method
tc	952.78	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=U375833&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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