2-[[(Dimethylamino)methylene]amino)-3-(3-chloro acid, methyl ester

Other names:	(E)-Methyl 3-(3-chloro-4-methoxyphenyl)-2-[[(dimethylamino)methylene]amino]propanoate 2-{[(Dimethylamino)methylene]amino}-3-(3-chloro-4-methyloxy-phenyl)propanoic acid, methyl ester (E)-Methyl 3-(3-chloro-4-methoxyphenyl)-2-{[(dimethylamino)methylene]amino}propanoate
Inchi:	InChI=1S/C14H19ClN2O3/c1-17(2)9-16-12(14(18)20-4)8-10-5-6-13(19-3)11(15)7-10/h5-
InchiKey:	RBQRRGQZLMOMPC-UHFFFAOYSA-N
Formula:	C14H19ClN2O3
SMILES:	COC(=O)C(Cc1ccc(OC)c(Cl)c1)N=CN(C)C
Mol. weight [g/mol]:	298.76

Physical Properties

Property code	Value	Unit	Source
hf	-366.99	kJ/mol	Joback Method
hvap	71.28	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.023		Crippen Method
mcvol	225.570	ml/mol	McGowan Method
pc	1783.35	kPa	Joback Method
rinpol	2187.00		NIST Webbook
rinpol	2187.00		NIST Webbook
tb	781.18	K	Joback Method
tc	998.64	K	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U378748&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