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

Other names: (E)-Ethyl 3-(3-chloro-4-ethoxyphenyl)-2-[[(dimethylamino)methylene]amino]propanoate
2-{[(Dimethylamino)methylene]amino}-3-(3-chloro-4-ethyloxy-phenyl)propanoic acid, ethyl ester
(E)-Ethyl 3-(3-chloro-4-ethoxyphenyl)-2-{[(dimethylamino)methylene]amino}propanoate

Inchi: InChI=1S/C16H23ClN2O3/c1-5-21-15-8-7-12(9-13(15)17)10-14(16(20)22-6-2)18-11-19(3

InchiKey: JQSFWELLVBCENF-UHFFFAOYSA-N

Formula: C16H23ClN2O3

SMILES: CCOC(=O)C(Cc1ccc(OCC)c(Cl)c1)N=CN(C)C

Mol. weight [g/mol]: 326.82

Physical Properties

Property code	Value	Unit	Source
hf	-408.27	kJ/mol	Joback Method
hvap	75.73	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.803		Crippen Method
mcvol	253.750	ml/mol	McGowan Method
pc	1525.88	kPa	Joback Method
rinpol	2277.00		NIST Webbook
rinpol	2277.00		NIST Webbook
tb	826.94	K	Joback Method
tc	1040.34	K	Joback Method

Sources

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=U378742&Units=SI

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

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