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

Other names: (E)-Butyl 3-(4-butoxy-3-chlorophenyl)-2-{[(dimethylamino)methylene]amino}propanoate
2-{[(Dimethylamino)methylene]amino}-3-(3-chloro-4-butyloxy-phenyl)propanoic acid, butyl ester
(E)-Butyl 3-(4-butoxy-3-chlorophenyl)-2-{[(dimethylamino)methylene]amino}propanoate

Inchi: InChI=1S/C20H31ClN2O3/c1-5-7-11-25-19-10-9-16(13-17(19)21)14-18(22-15-23(3)4)20(

InchiKey: AGTXJKSRRMGRQS-UHFFFAOYSA-N

Formula: C20H31ClN2O3

SMILES: CCCCOC(=O)C(Cc1ccc(OCCCC)c(Cl)c1)N=CN(C)C

Mol. weight [g/mol]: 382.93

Physical Properties

Property code	Value	Unit	Source
hf	-490.83	kJ/mol	Joback Method
hvap	84.63	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.363		Crippen Method
mcvol	310.110	ml/mol	McGowan Method
pc	1153.78	kPa	Joback Method
rinpol	2645.00		NIST Webbook
tb	918.46	K	Joback Method
tc	1131.74	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=U378741&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