

3,7-Dichloroquinoline-8-carboxylic acid, butyl ester

Other names:	3,7-Dichloroquinoline-8-carboxylic acid, n-butyl ester
Inchi:	InChI=1S/C14H13Cl2NO2/c1-2-3-6-19-14(18)12-11(16)5-4-9-7-10(15)8-17-13(9)12/h4-5
InchiKey:	NYAZOYGALCLHAE-UHFFFAOYSA-N
Formula:	C14H13Cl2NO2
SMILES:	CCCCOC(=O)c1c(Cl)ccc2cc(Cl)cnc12
Mol. weight [g/mol]:	298.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.91		Crippen Method
logp	4.498		Crippen Method
mcvol	206.800	ml/mol	McGowan Method
rinpol	2273.00		NIST Webbook
rinpol	2273.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373201&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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