7-Chloro-3-methyl-quinoline-8-carboxylic acid, butyl ester

Other names: 8-Quinolinecarboxylic acid, 7-chloro-3-methyl-, butyl ester
Inchi: InChI=1S/C15H16ClNO2/c1-3-4-7-19-15(18)13-12(16)6-5-11-8-10(2)9-17-14(11)13/h5-6
InchiKey: NKJJPSFPKYACSG-UHFFFAOYSA-N
Formula: C15H16ClNO2
SMILES: CCCCOC(=O)c1c(Cl)ccc2cc(C)cnc12
Mol. weight [g/mol]: 277.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.70		Crippen Method
logp	4.154		Crippen Method
mcvol	208.650	ml/mol	McGowan Method
rinpol	2267.00		NIST Webbook
rinpol	2267.00		NIST Webbook

Sources

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=U373135&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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