

# 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:** C<sub>15</sub>H<sub>16</sub>ClNO<sub>2</sub>

**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
rinpola	2267.00		NIST Webbook
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## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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/ci9903071>

## Legend

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

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