

Ethyl 5-chlorothiophene-2-carboxylate

Inchi:	InChI=1S/C7H7ClO2S/c1-2-10-7(9)5-3-4-6(8)11-5/h3-4H,2H2,1H3
InchiKey:	BMOKMXXT0ZFEIZ-UHFFFAOYSA-N
Formula:	C7H7ClO2S
SMILES:	CCOC(=O)c1ccc(Cl)s1
Mol. weight [g/mol]:	190.65
CAS:	5751-82-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.57		Crippen Method
logp	2.578		Crippen Method
mcvol	126.060	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5751826&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/68-223-9/Ethyl-5-chlorothiophene-2-carboxylate.pdf>

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