

3-Chlorobenzo[b]thiophene-2-carbonyl chloride

Inchi:	InChI=1S/C9H4Cl2OS/c10-7-5-3-1-2-4-6(5)13-8(7)9(11)12/h1-4H
InchiKey:	GWKSSMDJEWPKCM-UHFFFAOYSA-N
Formula:	C9H4Cl2OS
SMILES:	O=C(Cl)c1sc2ccccc2c1Cl
Mol. weight [g/mol]:	231.10
CAS:	21815-91-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.61		Crippen Method
logp	3.934		Crippen Method
mcvol	141.150	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=C21815918&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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