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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