

5-Chlorobenzo[b]thiophene-3-acetic acid

Inchi:	InChI=1S/C10H7ClO2S/c11-7-1-2-9-8(4-7)6(5-14-9)3-10(12)13/h1-2,4-5H,3H2,(H,12,13)
InchiKey:	QQKKTOPRRGBBCT-UHFFFAOYSA-N
Formula:	C10H7ClO2S
SMILES:	O=C(O)Cc1csc2ccc(Cl)cc12
Mol. weight [g/mol]:	226.68
CAS:	17266-30-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.62		Crippen Method
logp	3.182		Crippen Method
mcvol	148.870	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C17266307&Units=SI

Legend

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

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