

3-Chlorobenzo(b)thiophene-2-carboxylic acid

Inchi: InChI=1S/C9H5ClO2S/c10-7-5-3-1-2-4-6(5)13-8(7)9(11)12/h1-4H,(H,11,12)
InchiKey: HJTMIYKPPPYDRJ-UHFFFAOYSA-N
Formula: C9H5ClO2S
SMILES: O=C(O)c1sc2ccccc2c1Cl
Mol. weight [g/mol]: 212.65
CAS: 21211-22-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.78		Crippen Method
logp	3.253		Crippen Method
mccvol	134.780	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C21211223&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

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

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