

2-Chlorobenzo[b]thiophene-3-acetonitrile

Inchi:	InChI=1S/C10H6CINS/c11-10-8(5-6-12)7-3-1-2-4-9(7)13-10/h1-4H,5H2
InchiKey:	CBWNFQCLFYLDJQ-UHFFFAOYSA-N
Formula:	C10H6CINS
SMILES:	N#CCc1c(Cl)sc2ccccc12
Mol. weight [g/mol]:	207.68
CAS:	157549-49-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.39		Crippen Method
logp	3.621		Crippen Method
mcvol	142.810	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C157549490&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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
mcvol:	McGowan's characteristic volume

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