

3,4-Dibromo-2,5-dichlorothiophene

Inchi:	InChI=1S/C4Br2Cl2S/c5-1-2(6)4(8)9-3(1)7
InchiKey:	CQDQDBHWDGWKHL-UHFFFAOYSA-N
Formula:	C4Br2Cl2S
SMILES:	Clc1sc(Cl)c(Br)c1Br
Mol. weight [g/mol]:	310.82
CAS:	40477-45-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.92		Crippen Method
logp	4.580		Crippen Method
mcvol	123.590	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=C40477450&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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<https://www.chemeo.com/cid/22-927-8/3-4-Dibromo-2-5-dichlorothiophene.pdf>

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