

3-Bromo-2,5-dichlorothiophene

Inchi:	InChI=1S/C4HBrCl2S/c5-2-1-3(6)8-4(2)7/h1H
InchiKey:	PBUHOXBSIQJRNO-UHFFFAOYSA-N
Formula:	C4HBrCl2S
SMILES:	Clc1cc(Br)c(Cl)s1
Mol. weight [g/mol]:	231.93
CAS:	60404-18-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.76		Crippen Method
logp	3.817		Crippen Method
mcvol	106.090	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=C60404184&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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