

3,4-Bis-(p-chloro-phenyl)-thiophene

Inchi:	InChI=1S/C16H10Cl2S/c17-13-5-1-11(2-6-13)15-9-19-10-16(15)12-3-7-14(18)8-4-12/h1-
InchiKey:	QVBBMSVLQPYGII-UHFFFAOYSA-N
Formula:	C16H10Cl2S
SMILES:	Clc1ccc(-c2csc2-c2ccc(Cl)cc2)cc1
Mol. weight [g/mol]:	305.22
CAS:	116529-32-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.80		Crippen Method
logp	6.389		Crippen Method
mcvol	210.150	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116529329&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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