

3-Acetyl-2,5-dichlorothiophene

Other names:	2,5-Dichloro-3-thienyl methyl ketone Ethanone, 1-(2,5-dichloro-3-thienyl)- 1-(2,5-Dichloro-thiophen-3-yl)-ethanone 1-(2,5-dichloro-3-thienyl)ethan-1-one 2,5-DICHLORO-3-ACETYLTHIOPHENE
Inchi:	InChI=1S/C6H4Cl2OS/c1-3(9)4-2-5(7)10-6(4)8/h2H,1H3
InchiKey:	GYFDNIRENHZKGR-UHFFFAOYSA-N
Formula:	C6H4Cl2OS
SMILES:	CC(=O)c1cc(Cl)sc1Cl
Mol. weight [g/mol]:	195.07
CAS:	36157-40-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.26		Crippen Method
logp	3.257		Crippen Method
mcvol	118.340	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36157401&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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