

2-Iodo-5-methylthiophene

Inchi:	InChI=1S/C5H5IS/c1-4-2-3-5(6)7-4/h2-3H,1H3
InchiKey:	NAZNQEXKAPLVKC-UHFFFAOYSA-N
Formula:	C5H5IS
SMILES:	Cc1ccc(I)s1
Mol. weight [g/mol]:	224.06
CAS:	16494-36-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.85		Crippen Method
logp	2.661		Crippen Method
mcvol	104.020	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16494363&Units=SI

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/66-725-4/2-Iodo-5-methylthiophene.pdf>

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