

2,3'-Bithiophene

Other names:	2,3'-Bithienyl 2,3'-Dithienyl
Inchi:	InChI=1S/C8H6S2/c1-2-8(10-4-1)7-3-5-9-6-7/h1-6H
InchiKey:	ILQGHVXNYGLZSR-UHFFFAOYSA-N
Formula:	C8H6S2
SMILES:	c1csc(-c2ccsc2)c1
Mol. weight [g/mol]:	166.26
CAS:	2404-89-9

Physical Properties

Property code	Value	Unit	Source
ie	7.91	eV	NIST Webbook
log10ws	-3.59		Crippen Method
logp	3.477		Crippen Method
mcvol	117.360	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=C2404899&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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