

2,2'-Methylenedithiophene

Other names:	Bis(2-thienyl)methane Di-2-Thienylmethane Thiophene, 2,2'-methylenebis- Thiophene, 2,2'-methylenedi- 2,2'-Dithienylmethane
Inchi:	InChI=1S/C9H8S2/c1-3-8(10-5-1)7-9-4-2-6-11-9/h1-6H,7H2
InchiKey:	JZSRHKOFXIACDX-UHFFFAOYSA-N
Formula:	C9H8S2
SMILES:	c1csc(Cc2cccs2)c1
Mol. weight [g/mol]:	180.29
CAS:	4341-34-8

Physical Properties

Property code	Value	Unit	Source
ie	8.84	eV	NIST Webbook
ie	9.05	eV	NIST Webbook
log10ws	-3.09		Crippen Method
logp	3.400		Crippen Method
mvol	131.450	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=C4341348&Units=SI

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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