

3-vinylthiophene

Inchi:	InChI=1S/C6H6S/c1-2-6-3-4-7-5-6/h2-5H,1H2
InchiKey:	BOJMHBBWYPDQQH-UHFFFAOYSA-N
Formula:	C6H6S
SMILES:	C=Cc1ccsc1
Mol. weight [g/mol]:	110.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.05		Crippen Method
logp	2.391		Crippen Method
mcvol	87.990	ml/mol	McGowan Method
ripol	1332.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R301161&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/73-077-6/3-vinylthiophene.pdf>

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