

2-(1-Methylvinyl)thiophene

Other names:	Thiophene, 2-(1-methylethenyl)- 2-isopropenylthiophene
Inchi:	InChI=1S/C7H8S/c1-6(2)7-4-3-5-8-7/h3-5H,1H2,2H3
InchiKey:	FTMGWGRYZSQTMF-UHFFFAOYSA-N
Formula:	C7H8S
SMILES:	<chem>C=C(C)c1cccs1</chem>
Mol. weight [g/mol]:	124.20
CAS:	30616-73-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.47		Crippen Method
logp	2.781		Crippen Method
mcvol	102.080	ml/mol	McGowan Method
ripol	1433.00		NIST Webbook
ripol	1433.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30616730&Units=SI
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

Legend

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

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