

2-Thiopheneacrolein

Other names:	3-(2-thienyl)acrylaldehyde
Inchi:	InChI=1S/C7H6OS/c8-5-1-3-7-4-2-6-9-7/h1-6H/b3-1+
InchiKey:	IEAUKTACQUVNLS-HNQUOIGGSA-N
Formula:	C7H6OS
SMILES:	O=CC=Cc1cccs1
Mol. weight [g/mol]:	138.19
CAS:	14756-03-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.75		Crippen Method
logp	1.960		Crippen Method
mcvol	103.650	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=C14756037&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

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

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