

(2-Thienylthio)acetone

Inchi:	InChI=1S/C7H8OS2/c1-6(8)5-10-7-3-2-4-9-7/h2-4H,5H2,1H3
InchiKey:	YZNDRLAITXPMSG-UHFFFAOYSA-N
Formula:	C7H8OS2
SMILES:	CC(=O)CSc1cccs1
Mol. weight [g/mol]:	172.27
CAS:	41444-33-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.09		Crippen Method
logp	2.429		Crippen Method
mcvol	124.300	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=C41444331&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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<https://www.chemeo.com/cid/22-263-5/2-Thienylthio-acetone.pdf>

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