

1-Propanone, 1-(3-thienyl)

Other names:	3-Propionyl-thiophene 1-(3-thienyl)-1-propanone
Inchi:	InChI=1S/C7H8OS/c1-2-7(8)6-3-4-9-5-6/h3-5H,2H2,1H3
InchiKey:	QBCICFNKXBQWLN-UHFFFAOYSA-N
Formula:	C7H8OS
SMILES:	CCC(=O)c1ccsc1
Mol. weight [g/mol]:	140.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	2.341		Crippen Method
mcvol	107.950	ml/mol	McGowan Method
rinpol	1142.00		NIST Webbook
rinpol	1183.00		NIST Webbook
rinpol	1183.00		NIST Webbook

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=R90434&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/42-323-6/1-Propanone-1-3-thienyl.pdf>

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