

1-Hexanone, 1-(2-thienyl)-

Other names:	Ketone, pentyl 2-thienyl 2-Hexanoylthiophene 1-(2-Thienyl)-1-hexanone Thiophene, 2-hexanoyl
Inchi:	InChI=1S/C10H14OS/c1-2-3-4-6-9(11)10-7-5-8-12-10/h5,7-8H,2-4,6H2,1H3
InchiKey:	CVDZQNUYYOLFOO-UHFFFAOYSA-N
Formula:	C10H14OS
SMILES:	CCCCC(=O)c1cccs1
Mol. weight [g/mol]:	182.28
CAS:	26447-67-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.56		Crippen Method
logp	3.511		Crippen Method
mcvol	150.220	ml/mol	McGowan Method

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=C26447676&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/76-058-4/1-Hexanone-1-2-thienyl.pdf>

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