

2-Acetyl-5-nitrothiophene

Other names:	Ethanone, 1-(5-nitro-2-thienyl)- Thiophene, 2-acetyl-5-nitro-
Inchi:	InChI=1S/C6H5NO3S/c1-4(8)5-2-3-6(11-5)7(9)10/h2-3H,1H3
InchiKey:	CMXUIQITENCDDHH-UHFFFAOYSA-N
Formula:	C6H5NO3S
SMILES:	CC(=O)c1ccc([N+](=O)[O-])s1
Mol. weight [g/mol]:	171.17
CAS:	39565-00-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.54		Crippen Method
logp	1.859		Crippen Method
mcvol	111.280	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=C39565009&Units=SI

Legend

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

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