

# 2-Acetyl-5-chlorothiophene

<b>Other names:</b>	5-Chloro-2-thienyl methyl ketone Ethanone, 1-(5-chloro-2-thienyl)- Ketone, 5-chloro-2-thienyl methyl BA 11044 5-Chlor-2-acetyl thiophen 5-Chloro-2-acetyl thiophen 1-(5-Chloro-2-thienyl)ethanone 2-Chloro-5-acetylthiophene 5-Chloro-2-acetylthiophene NSC 43020 1-(5-chloro-2-thienyl)ethan-1-one
<b>Inchi:</b>	InChI=1S/C6H5ClOS/c1-4(8)5-2-3-6(7)9-5/h2-3H,1H3
<b>InchiKey:</b>	HTZGPEHWQCRXGZ-UHFFFAOYSA-N
<b>Formula:</b>	C6H5ClOS
<b>SMILES:</b>	CC(=O)c1ccc(Cl)s1
<b>Mol. weight [g/mol]:</b>	160.62
<b>CAS:</b>	6310-09-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.57		Crippen Method
logp	2.604		Crippen Method
mcvol	106.100	ml/mol	McGowan Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	390.70	K	2.30	NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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=C6310094&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**tbrp:** Boiling point at reduced pressure

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