

# 3-Acetyl-2-methyl-5-phenylthiophene

**Inchi:** InChI=1S/C13H12OS/c1-9(14)12-8-13(15-10(12)2)11-6-4-3-5-7-11/h3-8H,1-2H3  
**InchiKey:** GREAZYFTAJMZFD-UHFFFAOYSA-N  
**Formula:** C13H12OS  
**SMILES:** CC(=O)c1cc(-c2ccccc2)sc1C  
**Mol. weight [g/mol]:** 216.30  
**CAS:** 40932-63-6

## Physical Properties

Property code	Value	Unit	Source
hsub	108.90 ± 0.40	kJ/mol	NIST Webbook
log10ws	-4.97		Crippen Method
logp	3.926		Crippen Method
mvol	168.730	ml/mol	McGowan Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	107.30 ± 0.40	kJ/mol	330.00	NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=C40932636&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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