

# Thiophene, 2-pentanoyl

**Inchi:** InChI=1S/C9H12OS/c1-2-3-5-8(10)9-6-4-7-11-9/h4,6-7H,2-3,5H2,1H3  
**InchiKey:** KJMPCVRMAHTBR-UHFFFAOYSA-N  
**Formula:** C9H12OS  
**SMILES:** CCCCC(=O)c1cccs1  
**Mol. weight [g/mol]:** 168.26

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.14		Crippen Method
logp	3.121		Crippen Method
mcvol	136.130	ml/mol	McGowan Method
rinpol	1355.00		NIST Webbook
ripol	1993.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=U122192&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  
**ripol:** Polar retention indices

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