

3-Acetyl-2,5-dimethylthiophene

Other names:	Ethanone, 1-(2,5-dimethyl-3-thienyl)- Ketone, 2,5-dimethyl-3-thienyl methyl Dimethylthienylcetone 2,5-dimethylthiophen-3-yl methyl ketone
Inchi:	InChI=1S/C8H10OS/c1-5-4-8(6(2)9)7(3)10-5/h4H,1-3H3
InchiKey:	PUSJAEJRDNPYKM-UHFFFAOYSA-N
Formula:	C8H10OS
SMILES:	CC(=O)c1cc(C)sc1C
Mol. weight [g/mol]:	154.23
CAS:	2530-10-1

Physical Properties

Property code	Value	Unit	Source
hvap	61.30 ± 1.30	kJ/mol	NIST Webbook
log10ws	-2.84		Crippen Method
logp	2.568		Crippen Method
mcvol	122.040	ml/mol	McGowan Method
rinpol	1289.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2530101&Units=SI

Legend

hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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