

Ethanone, 1-(4-methyl-2-thienyl)-

Other names:	1-(4-Methyl-2-thienyl)ethanone 2-Acetyl-4-methylthiophene 1-(4-methyl-2-thienyl)ethan-1-one
Inchi:	InChI=1S/C7H8OS/c1-5-3-7(6(2)8)9-4-5/h3-4H,1-2H3
InchiKey:	NFZNHUNPIJPRMP-UHFFFAOYSA-N
Formula:	C7H8OS
SMILES:	CC(=O)c1cc(C)cs1
Mol. weight [g/mol]:	140.20
CAS:	13679-73-7

Physical Properties

Property code	Value	Unit	Source
hvap	63.00 ± 2.60	kJ/mol	NIST Webbook
log10ws	-2.36		Crippen Method
logp	2.259		Crippen Method
mcvol	107.950	ml/mol	McGowan Method
rinpol	1240.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13679737&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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