2-Acetyl-3-methylthiophene

Other names:	Ethanone, 1-(3-methyl-2-thienyl)-
	1-(3-Methyl-2-thienyl)ethanone
	3-Methyl-2-acetylthiophene
	Thiophene, 2-acetyl-3-methyl
	1-(3-methyl-2-thienyl)ethan-1-one
Inchi:	InChI=1S/C7H8OS/c1-5-3-4-9-7(5)6(2)8/h3-4H,1-2H3
InchiKey:	YBJDKNXEWQSGEL-UHFFFAOYSA-N
Formula:	C7H8OS
SMILES:	CC(=O)c1sccc1C
Mol. weight [g/mol]:	140.20
CAS:	13679-72-6

Physical Properties

Property code	Value	Unit	Source
hvap	57.10 ± 2.40	kJ/mol	NIST Webbook
log10ws	-2.36		Crippen Method
logp	2.259		Crippen Method
mcvol	107.950	ml/mol	McGowan Method
rinpol	1186.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1186.00		NIST Webbook
ripol	1760.00		NIST Webbook
ripol	1761.00		NIST Webbook
ripol	1762.00		NIST Webbook
ripol	1762.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C13679726&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
ripol:	Polar retention indices