

1-Propanone, 1-(5-methyl-2-thienyl)-

Other names:	2-Methyl-5-propionylthiophene 1-(2-Methyl-5-thienyl)-1-propanone Thiophene, 2-methyl-5-propionyl
Inchi:	InChI=1S/C8H10OS/c1-3-7(9)8-5-4-6(2)10-8/h4-5H,3H2,1-2H3
InchiKey:	ROPOMQPSWIOWSN-UHFFFAOYSA-N
Formula:	C8H10OS
SMILES:	CCC(=O)c1ccc(C)s1
Mol. weight [g/mol]:	154.23
CAS:	59303-13-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.78		Crippen Method
logp	2.649		Crippen Method
mcvol	122.040	ml/mol	McGowan Method
ripol	1280.00		NIST Webbook
ripol	1900.00		NIST Webbook
ripol	1900.00		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=C59303138&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

Latest version available from:

<https://www.cheméo.com/cid/60-030-1/1-Propanone-1-5-methyl-2-thienyl.pdf>

Generated by Cheméo on 2024-04-26 08:29:40.477840999 +0000 UTC m=+16409429.398418326.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.