1-Butanone, 1-(2-thienyl)-

Other names:	Ketone, propyl 2-thienyl
	2-Butyrylthiophene
	1-(2-Thienyl)-1-butanone
	n-Propyl 2-thienyl ketone
	2-n-Butyrylthiophene
	2-Butanoylthiophene
	1-(2-thienyl)butan-1-one
	Thiophene, 2-butanoyl
Inchi:	InChI=1S/C8H10OS/c1-2-4-7(9)8-5-3-6-10-8/h3,5-6H,2,4H2,1H3
InchiKey:	YXHIINNJOGKPLF-UHFFFAOYSA-N
Formula:	C8H10OS
SMILES:	CCCC(=O)c1cccs1
Mol. weight [g/mol]:	154.23
CAS:	5333-83-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.73		Crippen Method
logp	2.731		Crippen Method
mcvol	122.040	ml/mol	McGowan Method
rinpol	1252.00		NIST Webbook
rinpol	1252.00		NIST Webbook
ripol	1894.00		NIST Webbook
ripol	1894.00		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=C5333835&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