2-Propanone, 1-(3-thienyl)

Other names: 1-(3-thienyl)-2-propanone
Inchi: InChI=1S/C7H8OS/c1-6(8)4-7-2-3-9-5-7/h2-3,5H,4H2,1H3
InchiKey: CBKDLNBMOXQRLZ-UHFFFAOYSA-N
Formula: C7H8OS
SMILES: CC(=O)Cc1ccsc1
Mol. weight [g/mol]: 140.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.73		Crippen Method
logp	1.880		Crippen Method
mcvol	107.950	ml/mol	McGowan Method
rinpol	1134.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1134.00		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=R90523&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

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