

2-Propanone, 1-(2-thienyl)

Inchi: InChI=1S/C7H8OS/c1-6(8)5-7-3-2-4-9-7/h2-4H,5H2,1H3
InchiKey: FOWXQMONAFWJAD-UHFFFAOYSA-N
Formula: C7H8OS
SMILES: CC(=O)Cc1cccs1
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	1140.00		NIST Webbook
rinpol	1140.00		NIST Webbook

Sources

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=R69710&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/42-457-8/2-Propanone-1-2-thienyl.pdf>

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