3-methyl-2-(2-oxopropyl)thiophene

Inchi: InChI=1S/C8H10OS/c1-6-3-4-10-8(6)5-7(2)9/h3-4H,5H2,1-2H3
InchiKey: XDBOTNWICPQGCC-UHFFFAOYSA-N
Formula: C8H10OS
SMILES: CC(=O)Cc1sccc1C
Mol. weight [g/mol]: 154.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.21		Crippen Method
logp	2.188		Crippen Method
mcvol	122.040	ml/mol	McGowan Method
rinpol	1192.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R220121&Units=SI
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

Legend

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