Thiophene, 2-pentanoyl

Inchi: InChI=1S/C9H12OS/c1-2-3-5-8(10)9-6-4-7-11-9/h4,6-7H,2-3,5H2,1H3
InchiKey: KJMPRCVRMAHTBR-UHFFFAOYSA-N
Formula: C9H12OS
SMILES: CCCCC(=O)c1cccs1
Mol. weight [g/mol]: 168.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.14		Crippen Method
logp	3.121		Crippen Method
mcvol	136.130	ml/mol	McGowan Method
rinpol	1355.00		NIST Webbook
ripol	1993.00		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=U122192&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