1-(2-Furyl)-3-(2-thienyl)-2-propen-1-one

Other names: 2-Propen-1-one, 1-(2-furanyl)-3-(2-thienyl)-
Inchi: InChI=1S/C11H8O2S/c12-10(11-4-1-7-13-11)6-5-9-3-2-8-14-9/h1-8H/b6-5+
InchiKey: HIBLXINPOYYHFI-AATRIKPKSA-N
Formula: C11H8O2S
SMILES: O=C(C=Cc1cccs1)c1ccco1
Mol. weight [g/mol]: 204.25
CAS: 13343-95-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.68		Crippen Method
logp	3.237		Crippen Method
mcvol	146.420	ml/mol	McGowan Method

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=C13343958&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume