

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/ci9903071
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

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