4'-Methyl-3-(2-thienyl)acrylophenone

Other names:	1-(4-Methylphenyl)-3-(2-thienyl)-prop-2-en-1-one
	2-(2-Thienylidene)-4'-methylacetophenone
Inchi:	InChI=1S/C14H12OS/c1-11-4-6-12(7-5-11)14(15)9-8-13-3-2-10-16-13/h2-10H,1H3/b9-8+
InchiKey:	OUDDTWPBSXBJOY-CMDGGOBGSA-N
Formula:	C14H12OS
SMILES:	Cc1ccc(C(=O)C=Cc2cccs2)cc1
Mol. weight [g/mol]:	228.31
CAS:	6028-89-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.42		Crippen Method
logp	3.953		Crippen Method
mcvol	178.520	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6028893&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

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