

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

Other names:	2'-Thienylidene-4-nitroacetophenone 1-(4-Nitrophenyl)-3-(2-thienyl)-prop-2-en-1-one 1-(4-Nitrophenyl)-3-(2-thienyl)-2-propen-1-one
Inchi:	InChI=1S/C13H9NO3S/c15-13(8-7-12-2-1-9-18-12)10-3-5-11(6-4-10)14(16)17/h1-9H/b8-
InchiKey:	QZLINQZBUKTXIZ-BQYQJAHWSA-N
Formula:	C13H9NO3S
SMILES:	O=C(C=Cc1cccs1)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	259.28
CAS:	6028-92-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.59		Crippen Method
logp	3.552		Crippen Method
mcvol	181.850	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6028928&Units=SI
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

Legend

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

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