

1-(2-Naphthyl)-3-(2-thienyl)prop-2-en-1-one

Inchi:	InChI=1S/C17H12OS/c18-17(10-9-16-6-3-11-19-16)15-8-7-13-4-1-2-5-14(13)12-15/h1-12
InchiKey:	LAPXFVWYPUWTMF-MDZDMXLPSA-N
Formula:	C17H12OS
SMILES:	O=C(C=Cc1cccs1)c1ccc2ccccc2c1
Mol. weight [g/mol]:	264.34
CAS:	20894-63-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.75		Crippen Method
logp	4.797		Crippen Method
mcvol	201.330	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=C20894637&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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