

2-Thiopheneacetic acid, 2-naphthyl ester

Inchi:	InChI=1S/C16H12O2S/c17-16(11-15-6-3-9-19-15)18-14-8-7-12-4-1-2-5-13(12)10-14/h1-
InchiKey:	BRWGECRHSRQMIQ-UHFFFAOYSA-N
Formula:	C16H12O2S
SMILES:	O=C(Cc1cccs1)Oc1ccc2ccccc2c1
Mol. weight [g/mol]:	268.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.96		Crippen Method
logp	4.049		Crippen Method
mcvol	197.410	ml/mol	McGowan Method
rinpol	2307.00		NIST Webbook
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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=U308060&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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