

2-Thiopheneacetic acid, undec-2-enyl ester

Inchi:	InChI=1S/C17H26O2S/c1-2-3-4-5-6-7-8-9-10-13-19-17(18)15-16-12-11-14-20-16/h9-12,1
InchiKey:	AGFHZNSXSMDMHCS-MDZDMXLPSA-N
Formula:	C17H26O2S
SMILES:	CCCCCCCCC=CCOC(=O)Cc1cccs1
Mol. weight [g/mol]:	294.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.35		Crippen Method
logp	5.141		Crippen Method
mcvol	250.420	ml/mol	McGowan Method
rinpola	2133.00		NIST Webbook
rinpola	2133.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U299390&Units=SI

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/117-913-8/2-Thiopheneacetic-acid-undec-2-enyl-ester.pdf>

Generated by Cheméo on 2024-04-28 20:19:40.754539249 +0000 UTC m=+16624829.675116565.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.