2-Thiopheneacetic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

Inchi: InChI=1S/C16H20O2S/c1-12(2)7-8-14(10-13(3)4)18-16(17)11-15-6-5-9-19-15/h5-6,9,13-

InchiKey: UKBQFFHWLIDUGX-UHFFFAOYSA-N

Formula: C16H20O2S

SMILES: C=C(C)C#CC(CC(C)C)OC(=O)Cc1cccs1

Mol. weight [g/mol]: 276.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.60		Crippen Method
logp	3.828		Crippen Method
mcvol	227.730	ml/mol	McGowan Method
rinpol	1807.00		NIST Webbook
rinpol	1807.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299388&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

rinpol: Non-polar retention indices

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