2-Thiopheneacetic acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C17H22O2S/c1-5-7-14(4)16(10-9-13(2)3)19-17(18)12-15-8-6-11-20-15/h6,8,11

InchiKey: QKADLVHQHBTJMI-UHFFFAOYSA-N

Formula: C17H22O2S

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

Mol. weight [g/mol]: 290.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.02		Crippen Method
logp	4.218		Crippen Method
mcvol	241.820	ml/mol	McGowan Method
rinpol	1895.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299389&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