2-Thiopheneacetic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C14H14O2S/c1-10-6-11(2)8-12(7-10)16-14(15)9-13-4-3-5-17-13/h3-8H,9H2,1-

InchiKey: ZMHWEMOKWSYOSE-UHFFFAOYSA-N

Formula: C14H14O2S

SMILES: Cc1cc(C)cc(OC(=O)Cc2cccs2)c1

Mol. weight [g/mol]: 246.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.11		Crippen Method
logp	3.513		Crippen Method
mcvol	188.690	ml/mol	McGowan Method
rinpol	1903.00		NIST Webbook

Sources

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=U308055&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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