2-Thiopheneacetic acid, 3-methylphenyl ester

Inchi: InChI=1S/C13H12O2S/c1-10-4-2-5-11(8-10)15-13(14)9-12-6-3-7-16-12/h2-8H,9H2,1H3
InchiKey: DCTVPZAAAROBGF-UHFFFAOYSA-N
Formula: C13H12O2S
SMILES: Cc1cccc(OC(=O)Cc2cccs2)c1
Mol. weight [g/mol]: 232.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.63		Crippen Method
logp	3.205		Crippen Method
mcvol	174.600	ml/mol	McGowan Method
rinpol	1801.00		NIST Webbook
rinpol	1801.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U308053&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.