2-Thiophenecarboxylic acid, 3-methylphenyl ester

Inchi: InChI=1S/C12H10O2S/c1-9-4-2-5-10(8-9)14-12(13)11-6-3-7-15-11/h2-8H,1H3
InchiKey: KBQQRBXIAWUSAW-UHFFFAOYSA-N
Formula: C12H10O2S
SMILES: Cc1cccc(OC(=O)c2cccs2)c1
Mol. weight [g/mol]: 218.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.79		Crippen Method
logp	3.276		Crippen Method
mcvol	160.510	ml/mol	McGowan Method
rinpol	1752.00		NIST Webbook
rinpol	1752.00		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=U308061&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

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