2-Thiophenecarboxylic acid, 4-methoxyphenyl ester

Inchi: InChI=1S/C12H10O3S/c1-14-9-4-6-10(7-5-9)15-12(13)11-3-2-8-16-11/h2-8H,1H3
InchiKey: CIJQJYGRBZJGTF-UHFFFAOYSA-N
Formula: C12H10O3S
SMILES: COc1ccc(OC(=O)c2cccs2)cc1
Mol. weight [g/mol]: 234.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.44		Crippen Method
logp	2.976		Crippen Method
mcvol	166.380	ml/mol	McGowan Method
rinpol	1914.00		NIST Webbook
rinpol	1914.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U308064&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

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