2-Thiopheneacetic acid, 4-chlorophenyl ester

Inchi: InChI=1S/C12H9ClO2S/c13-9-3-5-10(6-4-9)15-12(14)8-11-2-1-7-16-11/h1-7H,8H2
InchiKey: JKMNFPKKWDGILK-UHFFFAOYSA-N
Formula: C12H9ClO2S
SMILES: O=C(Cc1cccs1)Oc1ccc(Cl)cc1
Mol. weight [g/mol]: 252.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.84		Crippen Method
logp	3.550		Crippen Method
mcvol	172.750	ml/mol	McGowan Method
rinpol	1889.00		NIST Webbook
rinpol	1889.00		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=U308054&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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