

2-Thiophenecarboxylic acid, 4-chlorophenyl ester

Inchi:	InChI=1S/C11H7ClO2S/c12-8-3-5-9(6-4-8)14-11(13)10-2-1-7-15-10/h1-7H
InchiKey:	RHDSCYYKAZNOCO-UHFFFAOYSA-N
Formula:	C11H7ClO2S
SMILES:	O=C(Oc1ccc(Cl)cc1)c1cccs1
Mol. weight [g/mol]:	238.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.00		Crippen Method
logp	3.621		Crippen Method
mcvol	158.660	ml/mol	McGowan Method
rinsol	1829.00		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=U308062&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinsol:	Non-polar retention indices

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