

2-Thiophenecarboxylic acid, 4-cyanophenyl ester

Inchi:	InChI=1S/C12H7NO2S/c13-8-9-3-5-10(6-4-9)15-12(14)11-2-1-7-16-11/h1-7H
InchiKey:	GUYZPPJEEMOMIM-UHFFFAOYSA-N
Formula:	C12H7NO2S
SMILES:	N#Cc1ccc(OC(=O)c2cccs2)cc1
Mol. weight [g/mol]:	229.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.67		Crippen Method
logp	2.839		Crippen Method
mcvol	161.890	ml/mol	McGowan Method
rinpol	1964.00		NIST Webbook
rinpol	1964.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308065&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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