

2-Thiopheneacetic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C13H9NO2S/c14-9-10-3-5-11(6-4-10)16-13(15)8-12-2-1-7-17-12/h1-7H,8H2
InchiKey: JBODTVOYLPKLIS-UHFFFAOYSA-N
Formula: C13H9NO2S
SMILES: N#Cc1ccc(OC(=O)Cc2cccs2)cc1
Mol. weight [g/mol]: 243.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.51		Crippen Method
logp	2.768		Crippen Method
mcvol	175.980	ml/mol	McGowan Method
rinpol	2006.00		NIST Webbook
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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=U308057&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
rinpol: Non-polar retention indices

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