

2-Thiopheneacetic acid, 4-methoxyphenyl ester

Inchi:	InChI=1S/C13H12O3S/c1-15-10-4-6-11(7-5-10)16-13(14)9-12-3-2-8-17-12/h2-8H,9H2,1H
InchiKey:	WTFWDIWIBJVIQV-UHFFFAOYSA-N
Formula:	C13H12O3S
SMILES:	COc1ccc(OC(=O)Cc2cccs2)cc1
Mol. weight [g/mol]:	248.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.28		Crippen Method
logp	2.905		Crippen Method
mcvol	180.470	ml/mol	McGowan Method
rinsol	1970.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308056&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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