

2-Thiopheneacetic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C12H9NO4S/c14-12(8-11-2-1-7-18-11)17-10-5-3-9(4-6-10)13(15)16/h1-7H,8H
InchiKey: IDOPUPRJKYPXNN-UHFFFAOYSA-N
Formula: C12H9NO4S
SMILES: O=C(Cc1cccs1)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 263.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	2.804		Crippen Method
mcvol	177.930	ml/mol	McGowan Method
rinpol	2140.00		NIST Webbook
rinpol	2140.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U308059&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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