2-Thiophenecarboxylic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C11H7NO4S/c13-11(10-2-1-7-17-10)16-9-5-3-8(4-6-9)12(14)15/h1-7H
InchiKey: QHJFYEJRQLKVEZ-UHFFFAOYSA-N
Formula: C11H7NO4S
SMILES: O=C(Oc1ccc([N+](=O)[O-])cc1)c1cccs1
Mol. weight [g/mol]: 249.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.97		Crippen Method
logp	2.876		Crippen Method
mcvol	163.840	ml/mol	McGowan Method
rinpol	2088.00		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=U308067&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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