

2-Thiophenecarboxylic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C13H12O2S/c1-9-6-10(2)8-11(7-9)15-13(14)12-4-3-5-16-12/h3-8H,1-2H3
InchiKey: KZBZXGUQWVMSAY-UHFFFAOYSA-N
Formula: C13H12O2S
SMILES: Cc1cc(C)cc(OC(=O)c2cccs2)c1
Mol. weight [g/mol]: 232.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.27		Crippen Method
logp	3.584		Crippen Method
mcvol	174.600	ml/mol	McGowan Method
rinpol	1855.00		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=U308063&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

Latest version available from:

<https://www.chemeo.com/cid/20-443-7/2-Thiophenecarboxylic-acid-3-5-dimethylphenyl-ester.pdf>

Generated by Cheméo on 2024-04-23 10:55:58.491268841 +0000 UTC m=+16159007.411846202.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.