

2-Thiophenecarboxylic acid, 3-methylphenyl ester

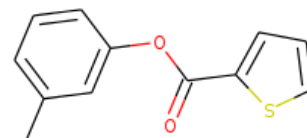
InChI: InChI=1S/C12H10O2S/c1-9-4-2-5-10(8-9)14-12(13)11-6-3-7-15-11/h2-8H,1H3

InChI Key: KBQQRBXIAWUSAW-UHFFFAOYSA-N

Formula: C12H10O2S

SMILES: Cc1cccc(OC(=O)c2cccs2)c1

Molecular Weight: 218.27



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	3.276		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H10O2S/c1-9-4-2-5-10\(8-9\)14-12\(13\)11-6-3-7-15-11-3-7-15-11/h2-8H,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H10O2S/c1-9-4-2-5-10(8-9)14-12(13)11-6-3-7-15-11-3-7-15-11/h2-8H,1H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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