

5-Methoxybenzofuran-2-carboxylic acid, ethyl ester

InChI: InChI=1S/C12H12O4/c1-3-15-12(13)11-7-8-6-9(14-2)4-5-10(8)16-11/h4-7H,3H2,1-2H3

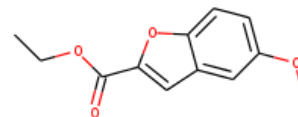
InChI Key: IJCODAOXFYTGBS-UHFFFAOYSA-N

Formula: C12H12O4

SMILES: CCOC(=O)c1cc2cc(OC)ccc2o1

Molecular Weight: 220.22

CAS: 50551-56-9



Physical Properties

| Property | Value | Unit | Source |
|---------------------------|-------|------|----------------|
| $\log P_{\text{oct/wat}}$ | 2.62 | | Crippen Method |

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H12O4/c1-3-15-12\(13\)11-7-8-6-9\(14-2\)4-5-10\(8\)16-11/h4-7H,3H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H12O4/c1-3-15-12(13)11-7-8-6-9(14-2)4-5-10(8)16-11/h4-7H,3H2,1-2H3)

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

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/85-609-2/5-Methoxybenzofuran-2-carboxylic%20acid%2C%20ethyl%20ester>

Generated by Cheméo on Thu, 15 Apr 2021 10:10:13 +0000.

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