

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
InchiKey:	IJCODAOXFYTGBS-UHFFFAOYSA-N
Formula:	C12H12O4
SMILES:	CCOC(=O)c1cc2cc(OC)ccc2o1
Mol. weight [g/mol]:	220.22
CAS:	50551-56-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.79		Crippen Method
logp	2.618		Crippen Method
mcvol	160.200	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C50551569&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/85-609-2/5-Methoxybenzofuran-2-carboxylic-acid-ethyl-ester.pdf>

Generated by Cheméo on 2025-12-05 20:13:48.304251658 +0000 UTC m=+4713825.834292312.

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