

7-Methoxybenzofuran-2-carboxylic acid, ethyl ester

Inchi:	InChI=1S/C12H12O4/c1-3-15-12(13)10-7-8-5-4-6-9(14-2)11(8)16-10/h4-7H,3H2,1-2H3
InchiKey:	SXCMZYVXJUJIDJ-UHFFFAOYSA-N
Formula:	C12H12O4
SMILES:	CCOC(=O)c1cc2cccc(OC)c2o1
Mol. weight [g/mol]:	220.22
CAS:	50551-58-1

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/ci9903071
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=C50551581&Units=SI

Legend

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

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