

3-Furancarboxylic acid, methyl ester

Other names:	3-Furoic acid, methyl ester Methyl 3-furancarboxylate Methyl 3-furoate Methyl furan-3-carboxylate NSC 305748
Inchi:	InChI=1S/C6H6O3/c1-8-6(7)5-2-3-9-4-5/h2-4H,1H3
InchiKey:	ZKHQSQYLKSSYIP-UHFFFAOYSA-N
Formula:	C6H6O3
SMILES:	<chem>COC(=O)c1ccoc1</chem>
Mol. weight [g/mol]:	126.11
CAS:	13129-23-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.45		Crippen Method
logp	1.066		Crippen Method
mcvol	89.250	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=C13129232&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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<https://www.chemeo.com/cid/81-030-8/3-Furancarboxylic-acid-methyl-ester.pdf>

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