

3-Methyl-2-furoic acid

Other names:	2-Furancarboxylic acid, 3-methyl-
Inchi:	InChI=1S/C6H6O3/c1-4-2-3-9-5(4)6(7)8/h2-3H,1H3,(H,7,8)
InchiKey:	BNYIQEFWGSXIKQ-UHFFFAOYSA-N
Formula:	C6H6O3
SMILES:	<chem>Cc1ccoc1C(=O)O</chem>
Mol. weight [g/mol]:	126.11
CAS:	4412-96-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.74		Crippen Method
logp	1.286		Crippen Method
mcvol	89.250	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4412968&Units=SI
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

Legend

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

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