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: Cc1ccoc1C(=O)O
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