

2-Methyl-3-furancarboxylic acid

Inchi:	InChI=1S/C6H6O3/c1-4-5(6(7)8)2-3-9-4/h2-3H,1H3,(H,7,8)
InchiKey:	CFGQZVOVFIZRMN-UHFFFAOYSA-N
Formula:	C6H6O3
SMILES:	Cc1occc1C(=O)O
Mol. weight [g/mol]:	126.11

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.74		Crippen Method
logp	1.286		Crippen Method
mcvol	89.250	ml/mol	McGowan Method
ripol	1655.00		NIST Webbook

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=R569258&Units=SI

Legend

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

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