

2-Furanpropionic acid

Other names:	2-Furanpropanoic acid furan-2-propionic acid
Inchi:	InChI=1S/C7H8O3/c8-7(9)4-3-6-2-1-5-10-6/h1-2,5H,3-4H2,(H,8,9)
InchiKey:	XLTJXJJMUFDQEZ-UHFFFAOYSA-N
Formula:	C7H8O3
SMILES:	O=C(O)CCc1ccco1
Mol. weight [g/mol]:	140.14
CAS:	935-13-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.53		Crippen Method
logp	1.297		Crippen Method
mcvol	103.340	ml/mol	McGowan Method

Sources

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=C935137&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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