

1,2-Ethanediol, 1-(2-furanyl)-

Other names:	1-(2-Furyl)-1,2-ethanediol 1-(2-Furanyl)-1,2-ethanediol
Inchi:	InChI=1S/C6H8O3/c7-4-5(8)6-2-1-3-9-6/h1-3,5,7-8H,4H2
InchiKey:	YOSOKWRRRCVPEJS-UHFFFAOYSA-N
Formula:	C6H8O3
SMILES:	OCC(O)c1ccco1
Mol. weight [g/mol]:	128.13
CAS:	19377-75-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.99		Crippen Method
logp	0.305		Crippen Method
mcvol	93.550	ml/mol	McGowan Method
rinpol	1099.00		NIST Webbook
rinpol	1099.00		NIST Webbook
ripol	2554.00		NIST Webbook

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=C19377754&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
rinpol:	Non-polar retention indices

ripol: Polar retention indices

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<https://www.chemeo.com/cid/32-600-9/1-2-Ethanediol-1-2-furanyl.pdf>

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