Isomaltol

Other names:	Ethanone, 1-(3-hydroxy-2-furanyl)-
	Ketone, 3-hydroxy-2-furyl methyl
	3-hydroxyfuran-2-yl methyl ketone
	2-Acetyl-3-hydroxyfuran
Inchi:	InChI=1S/C6H6O3/c1-4(7)6-5(8)2-3-9-6/h2-3,8H,1H3
InchiKey:	HPIGCVXMBGOWTF-UHFFFAOYSA-N
Formula:	C6H6O3
SMILES:	CC(=O)c1occc1O
Mol. weight [g/mol]:	126.11
CAS:	3420-59-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.41		Crippen Method
logp	1.188		Crippen Method
mcvol	89.250	ml/mol	McGowan Method
rinpol	995.00		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	978.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3420595&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices