

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/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/92-467-2/Isomaltol.pdf>

Generated by Cheméo on 2024-04-30 17:30:46.446356802 +0000 UTC m=+16787495.366934115.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.