4H-Pyran-4-one, 3,5-dihydroxy-2-methyl-

Other names:	3,5-Dihydroxy-2-methyl-4-pyrone
	3,5-Dihydroxy-2-methyl-4H-pyran-4-one
	5-Hydroxymaltol
	2-Methyl-3,5-dihydroxy-4H-pyran-4-one
	3,5-Dihydroxy-6-methyl-4-pyrone
	Hydroxymaltol
	3,5-Dihydroxy-2-methyl-4H-pyran-4-one (hydroxymaltol)
	3,5-Dihydroxy-6-methyl-4H-pyran-4-one
Inchi:	InChI=1S/C6H6O4/c1-3-5(8)6(9)4(7)2-10-3/h2,7-8H,1H3
InchiKey:	SSSNQLHKSUJJTE-UHFFFAOYSA-N
Formula:	C6H6O4
SMILES:	Cc1occ(O)c(=O)c1O
Mol. weight [g/mol]:	142.11
CAS:	1073-96-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Crippen Method
logp	0.359		Crippen Method
mcvol	95.120	ml/mol	McGowan Method
rinpol	1188.30		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1197.00		NIST Webbook
rinpol	1189.00		NIST Webbook
rinpol	1187.00		NIST Webbook
rinpol	1205.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1220.00		NIST Webbook
ripol	2295.00		NIST Webbook
ripol	2271.00		NIST Webbook
ripol	2295.00		NIST Webbook
ripol	2294.00		NIST Webbook
ripol	2233.00		NIST Webbook
ripol	2309.00		NIST Webbook
ripol	2295.00		NIST Webbook
ripol	2271.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1073967&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
ripol:	Polar retention indices