

4H-Pyran-4-one, 5-hydroxy-2-(hydroxymethyl)-

Other names:	Kojic acid 5-Hydroxy-2-(hydroxymethyl)-4-pyrone 5-Hydroxy-2-hydroxymethyl-4H-pyran-4-one Pyran-4-one, 5-hydroxy-2-(hydroxymethyl)
Inchi:	InChI=1S/C6H6O4/c7-2-4-1-5(8)6(9)3-10-4/h1,3,7,9H,2H2
InchiKey:	BEJNERDRQOWKJM-UHFFFAOYSA-N
Formula:	C6H6O4
SMILES:	O=c1cc(CO)occ1O
Mol. weight [g/mol]:	142.11
CAS:	501-30-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.32		Crippen Method
logp	-0.162		Crippen Method
mcvol	95.120	ml/mol	McGowan Method
rinpol	1192.10		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C501304&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

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