

4H-Pyran-4-one, 5-hydroxy-2-methyl-

Other names:	Allomaltol Kojic acid, «alpha»-deoxy- 5-Hydroxy-2-methyl-«gamma»-pyrone 5-Hydroxy-2-methyl-4H-pyran-4-one 2-Methyl-5-hydroxy-4H-pyran-4-one
Inchi:	InChI=1S/C6H6O3/c1-4-2-5(7)6(8)3-9-4/h2-3,8H,1H3
InchiKey:	IQXWFHDFTA ZGNB-UHFFFAOYSA-N
Formula:	C6H6O3
SMILES:	<chem>Cc1cc(=O)c(O)co1</chem>
Mol. weight [g/mol]:	126.11
CAS:	644-46-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.65		Crippen Method
logp	0.654		Crippen Method
mcvol	89.250	ml/mol	McGowan Method
rinpol	1139.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1139.00		NIST Webbook
ripol	2030.00		NIST Webbook
ripol	2030.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C644462&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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