

2H-Pyran-2-one, 4,6-dimethyl-

Other names:	Sorbic acid, 5-hydroxy-3-methyl-, «delta»-lactone Mesitene lactone 2,4-Dimethyl-«alpha»-pyrone 4,6-Dimethyl-«alpha»-pyrone 4,6-Dimethyl-2-pyrone 4,6-Dimethylcoumalin 4,6-Dimethyl-2H-pyran-2-one
Inchi:	InChI=1S/C7H8O2/c1-5-3-6(2)9-7(8)4-5/h3-4H,1-2H3
InchiKey:	IXYLIUKQQQXXON-UHFFFAOYSA-N
Formula:	C7H8O2
SMILES:	<chem>Cc1cc(C)oc(=O)c1</chem>
Mol. weight [g/mol]:	124.14
CAS:	675-09-2

Physical Properties

Property code	Value	Unit	Source
ie	8.51	eV	NIST Webbook
log10ws	-5.58		Crippen Method
logp	1.257		Crippen Method
mcvol	97.470	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C675092&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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