5-hydroxy-6-methyl-(2H)-pyran-2-one

Inchi: InChI=1S/C6H6O3/c1-4-5(7)2-3-6(8)9-4/h2-3,7H,1H3
InchiKey: AFRWGSJXXLIKEI-UHFFFAOYSA-N
Formula: C6H6O3
SMILES: Cc1oc(=O)ccc1O
Mol. weight [g/mol]: 126.11

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	1040.00		NIST Webbook
ripol	2119.00		NIST Webbook
ripol	2119.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R225988&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

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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