

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/ci990307I>
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

Latest version available from:

<https://www.cheméo.com/cid/11-951-3/5-hydroxy-6-methyl-2H-pyran-2-one.pdf>

Generated by Cheméo on 2024-04-25 16:50:31.187424957 +0000 UTC m=+16353080.108002268.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.