

4-Methyl-5,6-dihydropyran-2-one

Inchi: InChI=1S/C6H6O2/c1-5-2-3-8-6(7)4-5/h2-4H,1H3
InchiKey: FINYGTPXELVTLO-UHFFFAOYSA-N
Formula: C6H6O2
SMILES: Cc1ccoc(=O)c1
Mol. weight [g/mol]: 110.11

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.10		Crippen Method
logp	0.948		Crippen Method
mcvol	83.380	ml/mol	McGowan Method
ripol	2027.00		NIST Webbook
ripol	2027.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R610356&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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

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<https://www.chemeo.com/cid/81-029-0/4-Methyl-5-6-dihydropyran-2-one.pdf>

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