

2-Acetyl-3-hydroxypyran-4-one

Inchi: InChI=1S/C7H6O4/c1-4(8)7-6(10)5(9)2-3-11-7/h2-3,10H,1H3
InchiKey: CDKPTINNZGFVEO-UHFFFAOYSA-N
Formula: C7H6O4
SMILES: CC(=O)c1occc(=O)c1O
Mol. weight [g/mol]: 154.12

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.84		Crippen Method
logp	0.548		Crippen Method
mcvol	104.910	ml/mol	McGowan Method
ripol	1395.00		NIST Webbook
ripol	1395.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R531832&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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