3,6-Dimethyl-2H-pyran -2-one

Inchi: InChI=1S/C7H8O2/c1-5-3-4-6(2)9-7(5)8/h3-4H,1-2H3
InchiKey: LTLJMIDAHYUFMI-UHFFFAOYSA-N
Formula: C7H8O2
SMILES: Cc1ccc(C)c(=O)o1
Mol. weight [g/mol]: 124.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.58		Crippen Method
logp	1.257		Crippen Method
mcvol	97.470	ml/mol	McGowan Method
ripol	2152.00		NIST Webbook
ripol	2152.00		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=R519085&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

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