1,3-Dioxol-2-one,4,5-dimethyl-

Inchi: InChI=1S/C5H6O3/c1-3-4(2)8-5(6)7-3/h1-2H3
InchiKey: QYIOFABFKUOIBV-UHFFFAOYSA-N
Formula: C5H6O3
SMILES: Cc1oc(=O)oc1C
Mol. weight [g/mol]: 114.10
CAS: 37830-90-3

Physical Properties

Property code	Value	Unit	Source
ie	9.10	eV	NIST Webbook
log10ws	-9.31		Crippen Method
logp	0.850		Crippen Method
mcvol	79.460	ml/mol	McGowan Method

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=C37830903&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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