4,5-DIMETHYL-1,3-DIOXOL-2-ONE

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

Physical Properties

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

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C37830903&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume