

1,3-Dioxolan-2-one, 4,5-bis(methylene)-

Inchi: InChI=1S/C5H4O3/c1-3-4(2)8-5(6)7-3/h1-2H2
InchiKey: YJPJOELHSKMFPG-UHFFFAOYSA-N
Formula: C5H4O3
SMILES: C=c1oc(=O)oc1=C
Mol. weight [g/mol]: 112.08
CAS: 62458-20-2

Physical Properties

Property code	Value	Unit	Source
ie	9.30	eV	NIST Webbook
log10ws	-7.82		Crippen Method
logp	-0.947		Crippen Method
mcvol	75.160	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C62458202&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.chemeo.com/cid/88-090-5/1-3-Dioxolan-2-one-4-5-bis-methylene.pdf>

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