Hydroxycarbonyl-d1

Inchi: InChI=1S/CHO2/c2-1-3/h(H,2,3)/i/hD
InchiKey: ORTFAQDWJHRMNX-DYCDLGHISA-N
Formula: CDO2
SMILES: O=[C]O
Mol. weight [g/mol]: 46.02
CAS: 90965-57-4

Physical Properties

Property code	Value	Unit	Source
ea	1.51 ± 0.01	eV	NIST Webbook
ea	1.37 ± 0.01	eV	NIST Webbook
log10ws	-3.93		Crippen Method
logp	-0.388		Crippen Method
mcvol	30.240	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C90965574&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

ea: Electron affinity
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume