1-Oxoprop-2-enyl

Other names: Propenoyl radical
Inchi: InChI=1S/C3H3O/c1-2-3-4/h2H,1H2
InchiKey: LVOICKNPHXSSQM-UHFFFAOYSA-N
Formula: C3H3O
SMILES: C=C[C]=O
Mol. weight [g/mol]: 55.06
CAS: 72241-20-4

Physical Properties

Property code	Value	Unit	Source
ie	7.00	eV	NIST Webbook
log10ws	-4.80		Crippen Method
logp	0.282		Crippen Method
mcvol	48.250	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C72241204&Units=SI

Legend

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