

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

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<https://www.chemeo.com/cid/77-921-4/1-Oxoprop-2-enyl.pdf>

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