

Propanoyl

Other names:	Propionyl radical
Inchi:	InChI=1S/C3H5O/c1-2-3-4/h2H2,1H3
InchiKey:	UFUASNAHBMBJIX-UHFFFAOYSA-N
Formula:	C3H5O
SMILES:	CC[C]=O
Mol. weight [g/mol]:	57.07
CAS:	15843-24-0

Physical Properties

Property code	Value	Unit	Source
ea	1.91 ± 0.15	eV	NIST Webbook
ea	3.51	eV	NIST Webbook
ie	6.60	eV	NIST Webbook
log10ws	-4.95		Crippen Method
logp	0.506		Crippen Method
mcvol	52.550	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15843240&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
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/34-731-2/Propanoyl.pdf>

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