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