EtCO2 anion

Inchi: InChI=1S/C3H6O2/c1-2-3(4)5/h2H2,1H3,(H,4,5)/p-1
InchiKey: XBDQKXXYIPTUBI-UHFFFAOYSA-M
Formula: C3H5O2-
SMILES: CCC(=O)[O-]
Mol. weight [g/mol]: 73.07
CAS: 72-03-7

Physical Properties

Property code	Value	Unit	Source
ean	3.43 ± 0.16	eV	NIST Webbook
ean	3.40 ± 0.30	eV	NIST Webbook
log10ws	-2.88		Crippen Method
logp	-0.854		Crippen Method
mcvol	58.420	ml/mol	McGowan Method

Sources

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=C72037&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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