iPrCO2 anion

Inchi: InChI=1S/C4H8O2/c1-3(2)4(5)6/h3H,1-2H3,(H,5,6)/p-1
InchiKey: KQNPFQTWMSNSAP-UHFFFAOYSA-M
Formula: C4H7O2-
SMILES: CC(C)C(=O)[O-]
Mol. weight [g/mol]: 87.10
CAS: 5711-69-3

Physical Properties

Property code	Value	Unit	Source
ean	3.50 ± 0.16	eV	NIST Webbook
log10ws	-3.06		Crippen Method
logp	-0.608		Crippen Method
mcvol	72.510	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=C5711693&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.