

MeCO2 anion

Inchi: InChI=1S/C2H4O2/c1-2(3)4/h1H3,(H,3,4)/p-1
InchiKey: QTBSBXVTEAMEQO-UHFFFAOYSA-M
Formula: C2H3O2-
SMILES: CC(=O)[O-]
Mol. weight [g/mol]: 59.04
CAS: 71-50-1

Physical Properties

Property code	Value	Unit	Source
ean	3.40 ± 0.30	eV	NIST Webbook
ean	3.18 ± 0.05	eV	NIST Webbook
ean	3.30 ± 0.20	eV	NIST Webbook
ean	3.25 ± 0.01	eV	NIST Webbook
ean	3.38 ± 0.05	eV	NIST Webbook
ean	3.47 ± 0.01	eV	NIST Webbook
log10ws	-2.46		Crippen Method
logp	-1.244		Crippen Method
mcpvol	44.330	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=C71501&Units=SI>

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

Latest version available from:

<https://www.chemeo.com/cid/55-561-8/MeCO2-anion.pdf>

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