

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

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[https://www.chemeo.com/cid/34-116-5/EtCO₂-anion.pdf](https://www.chemeo.com/cid/34-116-5/EtCO2-anion.pdf)

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