

ClCH₂CO₂ anion

Inchi: InChI=1S/C2H3ClO2/c3-1-2(4)5/h1H2,(H,4,5)/p-1
InchiKey: FOCAUTSVDIKZOP-UHFFFAOYSA-M
Formula: C₂H₂ClO₂⁻
SMILES: O=C([O-])CCl
Mol. weight [g/mol]: 93.49
CAS: 14526-03-5

Physical Properties

Property code	Value	Unit	Source
ean	3.93 ± 0.03	eV	NIST Webbook
ean	3.91 ± 0.16	eV	NIST Webbook
log10ws	-2.61		Crippen Method
logp	-1.025		Crippen Method
mcvol	56.570	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C14526035&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/38-796-7/ClCH₂CO₂-anion.pdf](https://www.chemeo.com/cid/38-796-7/ClCH2CO2-anion.pdf)

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