

ICH₂CO₂ anion

Inchi:	InChI=1S/C2H3IO2/c3-1-2(4)5/h1H2,(H,4,5)/p-1
InchiKey:	JDNTWHVOXJZDSN-UHFFFAOYSA-M
Formula:	C2H2IO2-
SMILES:	O=C([O-])Cl
Mol. weight [g/mol]:	184.94
CAS:	152-34-1

Physical Properties

Property code	Value	Unit	Source
ean	3.99 ± 0.16	eV	NIST Webbook
log10ws	-3.41		Crippen Method
logp	-0.829		Crippen Method
mcvol	70.150	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=C152341&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/61-977-0/ICH2CO2-anion.pdf>

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