

MeCH(OH)CO₂ anion

Inchi:	InChI=1S/C3H6O3/c1-2(4)3(5)6/h2,4H,1H3,(H,5,6)/p-1
InchiKey:	JVTAAEKCFNVCJ-UHFFFAOYSA-M
Formula:	C ₃ H ₅ O ₃ ⁻
SMILES:	CC(O)C(=O)[O-]
Mol. weight [g/mol]:	89.07
CAS:	113-21-3

Physical Properties

Property code	Value	Unit	Source
ean	3.86 ± 0.16	eV	NIST Webbook
log10ws	-2.25		Crippen Method
logp	-1.883		Crippen Method
mcvol	64.290	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=C113213&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/12-931-4/MeCH-OH-CO2-anion.pdf>

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