

CH₃C(O)OO

Other names:	CH ₃ COO ₂
Inchi:	InChI=1S/C ₂ H ₃ O ₃ /c1-2(3)5-4/h1H ₃
InchiKey:	ZBQKPDHUDKSCRS-UHFFFAOYSA-N
Formula:	C ₂ H ₃ O ₃
SMILES:	CC(=O)O[O]
Mol. weight [g/mol]:	75.04
CAS:	36709-10-1

Physical Properties

Property code	Value	Unit	Source
log ₁₀ ws	-4.40		Crippen Method
logp	-0.105		Crippen Method
mcvol	50.200	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=C36709101&Units=SI

Legend

log ₁₀ ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.cheméo.com/cid/11-604-8/CH3C-O-OO.pdf>

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