(CH3)3CO2

Inchi: InChI=1S/C4H9O2/c1-4(2,3)6-5/h1-3H3
InchiKey: YKTNISGZEGZHIS-UHFFFAOYSA-N
Formula: C4H9O2
SMILES: CC(C)(C)O[O]
Mol. weight [g/mol]: 89.11
CAS: 3395-62-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.58		Crippen Method
logp	1.147		Crippen Method
mcvol	76.810	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C3395628&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume