CF3CO2 anion

Inchi: InChI=1S/C2HF3O2/c3-2(4,5)1(6)7/h(H,6,7)/p-1
InchiKey: DTQVDTLACAAQTR-UHFFFAOYSA-M
Formula: C2F3O2-
SMILES: O=C([O-])C(F)(F)F
Mol. weight [g/mol]: 113.02
CAS: 14477-72-6

Physical Properties

Property code	Value	Unit	Source
ean	4.46 ± 0.18	eV	NIST Webbook
log10ws	-3.12		Crippen Method
logp	-0.701		Crippen Method
mcvol	49.640	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=C14477726&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.