

Hydrocarboxyl radical

Inchi:	InChI=1S/CHO2/c2-1-3/h(H,2,3)
InchiKey:	ORTFAQDWJHRMNX-UHFFFAOYSA-N
Formula:	CHO2
SMILES:	O=[C]O
Mol. weight [g/mol]:	45.02
CAS:	2564-86-5

Physical Properties

Property code	Value	Unit	Source
affp	623.40	kJ/mol	NIST Webbook
basg	590.90	kJ/mol	NIST Webbook
ea	3.54 ± 0.11	eV	NIST Webbook
ea	3.50 ± 0.01	eV	NIST Webbook
ea	2.18 ± 0.02	eV	NIST Webbook
ea	1.18	eV	NIST Webbook
ea	1.51 ± 0.01	eV	NIST Webbook
ea	1.38 ± 0.01	eV	NIST Webbook
ea	3.50 ± 0.00	eV	NIST Webbook
hfp _i	597.00 ± 8.00	kJ/mol	NIST Webbook
hfp _{iz}	590.00 ± 8.00	kJ/mol	NIST Webbook
ie	8.49 ± 0.01	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
log10ws	-3.93		Crippen Method
logp	-0.388		Crippen Method
mcvol	30.240	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=C2564865&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
ea:	Electron affinity
hfpi:	Enthalpy of formation of positive ion at standard conditions
hfpiz:	Enthalpy of formation of positive ion at 0K
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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