

Trichloromethyl radical

Inchi:	InChI=1S/CCl3/c2-1(3)4
InchiKey:	ZBZJXHCVGLJWFG-UHFFFAOYSA-N
Formula:	CCl3
SMILES:	Cl[C](Cl)Cl
Mol. weight [g/mol]:	118.37
CAS:	3170-80-7

Physical Properties

Property code	Value	Unit	Source
ea	2.58 ± 0.20	eV	NIST Webbook
ea	2.10 ± 0.35	eV	NIST Webbook
ea	1.89	eV	NIST Webbook
ea	2.19 ± 0.27	eV	NIST Webbook
ea	2.16 ± 0.10	eV	NIST Webbook
ea	1.44 ± 0.05	eV	NIST Webbook
ea	1.30 ± 0.30	eV	NIST Webbook
ie	8.11 ± 0.01	eV	NIST Webbook
ie	8.78 ± 0.05	eV	NIST Webbook
ie	8.28	eV	NIST Webbook
ie	8.70 ± 0.10	eV	NIST Webbook
ie	8.11 ± 0.01	eV	NIST Webbook
ie	8.06 ± 0.02	eV	NIST Webbook
log10ws	-1.80		Crippen Method
logp	2.150		Crippen Method
mcvol	59.520	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=C3170807&Units=SI

Legend

ea:	Electron affinity
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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