Chlorofluoromethylene

Inchi: InChI=1S/CClF/c2-1-3
InchiKey: KYKAJFCTULSVSH-UHFFFAOYSA-N
Formula: CClF
SMILES: F[C]Cl
Mol. weight [g/mol]: 66.46
CAS: 1691-88-9

Physical Properties

Property code	Value	Unit	Source
affp	772.40	kJ/mol	NIST Webbook
basg	740.00	kJ/mol	NIST Webbook
ie	12.00 ± 1.00	eV	NIST Webbook
ie	10.70	eV	NIST Webbook
ie	10.62	eV	NIST Webbook
log10ws	-0.80		Crippen Method
logp	1.191		Crippen Method
mcvol	34.660	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1691889&Units=SI
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

Legend

affp: Proton affinity
basg: Gas basicity
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume