

Chloromethylene

Inchi: InChI=1S/CHCl/c1-2/h1H
InchiKey: LKYXEULZVGJVTG-UHFFFAOYSA-N
Formula: CHCl
SMILES: [CH]Cl
Mol. weight [g/mol]: 48.47
CAS: 2108-20-5

Physical Properties

Property code	Value	Unit	Source
affp	874.10	kJ/mol	NIST Webbook
basg	839.90	kJ/mol	NIST Webbook
ea	1.21 ± 0.01	eV	NIST Webbook
ea	1.21 ± 0.01	eV	NIST Webbook
ie	9.84	eV	NIST Webbook
log10ws	-0.45		Crippen Method
logp	0.894		Crippen Method
mcvol	32.890	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=C2108205&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

affp: Proton affinity
basg: Gas basicity
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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