

Dichloromethylene

Inchi: InChI=1S/CCl2/c2-1-3
InchiKey: PFBUKDPBVNJDEW-UHFFFAOYSA-N
Formula: CCl2
SMILES: Cl[C]Cl
Mol. weight [g/mol]: 82.92
CAS: 1605-72-7

Physical Properties

Property code	Value	Unit	Source
affp	861.00	kJ/mol	NIST Webbook
basg	828.50	kJ/mol	NIST Webbook
ea	1.59 ± 0.01	eV	NIST Webbook
ea	1.66 ± 0.14	eV	NIST Webbook
ea	1.59 ± 0.07	eV	NIST Webbook
ea	1.60 ± 0.01	eV	NIST Webbook
ea	2.50 ± 0.60	eV	NIST Webbook
ea	1.80 ± 0.30	eV	NIST Webbook
ie	9.27 ± 0.04	eV	NIST Webbook
ie	9.76	eV	NIST Webbook
log10ws	-1.10		Crippen Method
logp	1.460		Crippen Method
mcvol	45.130	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C1605727&Units=SI>

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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