

Methylene, bromochloro-

Inchi:	InChI=1S/CBrCl/c2-1-3
InchiKey:	CUTIHTZEPAAEMS-UHFFFAOYSA-N
Formula:	CBrCl
SMILES:	Cl[C]Br
Mol. weight [g/mol]:	127.37
CAS:	13590-47-1

Physical Properties

Property code	Value	Unit	Source
ie	10.00 ± 1.00	eV	NIST Webbook
log10ws	-1.37		Crippen Method
logp	1.616		Crippen Method
mcvol	50.390	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=C13590471&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/53-124-5/Methylene-bromochloro.pdf>

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