

1,3-Cyclohexadien-5-yne, 1,2,3,4-tetrachloro-

Inchi: InChI=1S/C6Cl4/c7-3-1-2-4(8)6(10)5(3)9
InchiKey: CGJZVCVOGNJABT-UHFFFAOYSA-N
Formula: C6Cl4
SMILES: Clc1c#cc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 213.88
CAS: 13280-72-3

Physical Properties

Property code	Value	Unit	Source
ie	10.70 ± 0.20	eV	NIST Webbook
log10ws	-3.58		Crippen Method
logp	3.901		Crippen Method
mcvol	116.300	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C13280723&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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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<https://www.chemeo.com/cid/77-860-2/1-3-Cyclohexadien-5-yne-1-2-3-4-tetrachloro.pdf>

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