

1,3-Cyclohexadien-5-yne,1,4-dichloro-

Inchi: InChI=1S/C6H2Cl2/c7-5-1-2-6(8)4-3-5/h1-2H
InchiKey: BMCWIYJTZUFEDG-UHFFFAOYSA-N
Formula: C6H2Cl2
SMILES: Clc1c#cc(Cl)cc1
Mol. weight [g/mol]: 144.99
CAS: 73513-56-1

Physical Properties

Property code	Value	Unit	Source
ie	9.10 ± 0.20	eV	NIST Webbook
log10ws	-2.21		Crippen Method
logp	2.594		Crippen Method
mcvol	91.820	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=C73513561&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/12-816-2/1-3-Cyclohexadien-5-yne-1-4-dichloro.pdf>

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