

1,3-Cyclohexadien-5-yne,1,2-dichloro-

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|-----------------------------|---|
| Inchi: | InChI=1S/C6H2Cl2/c7-5-3-1-2-4-6(5)8/h1,3H |
| InchiKey: | SDOVMOUWFIZPCZ-UHFFFAOYSA-N |
| Formula: | C6H2Cl2 |
| SMILES: | C1C=C=C=CC=C1Cl |
| Mol. weight [g/mol]: | 144.99 |
| CAS: | 24634-92-2 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|-------------|--------|----------------|
| ie | 9.70 ± 0.20 | eV | NIST Webbook |
| log10ws | -2.98 | | Crippen Method |
| logp | 2.556 | | Crippen Method |
| mcvol | 91.820 | 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=C24634922&Units=SI |

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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