

2H-Pyran, tetrahydro, 2,6-dichloro, # 1

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|----------------------|--|
| Inchi: | InChI=1S/C5H8Cl2O/c6-4-2-1-3-5(7)8-4/h4-5H,1-3H2 |
| InchiKey: | VPNYLBRZFCLADG-UHFFFAOYSA-N |
| Formula: | C5H8Cl2O |
| SMILES: | C1C1CCCC(Cl)O1 |
| Mol. weight [g/mol]: | 155.02 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -102.02 | kJ/mol | Joback Method |
| hf | -276.03 | kJ/mol | Joback Method |
| hfus | 17.98 | kJ/mol | Joback Method |
| hvap | 40.12 | kJ/mol | Joback Method |
| log10ws | -2.42 | | Crippen Method |
| logp | 2.317 | | Crippen Method |
| mcvol | 100.800 | ml/mol | McGowan Method |
| pc | 3862.67 | kPa | Joback Method |
| rinpol | 1080.00 | | NIST Webbook |
| tb | 430.49 | K | Joback Method |
| tc | 653.29 | K | Joback Method |
| tf | 235.66 | K | Joback Method |
| vc | 0.366 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 181.00 | J/molxK | 430.49 | Joback Method |
| cpg | 193.57 | J/molxK | 467.62 | Joback Method |
| cpg | 205.47 | J/molxK | 504.76 | Joback Method |
| cpg | 216.69 | J/molxK | 541.89 | Joback Method |
| cpg | 227.26 | J/molxK | 579.02 | Joback Method |
| cpg | 237.19 | J/molxK | 616.16 | Joback Method |
| cpg | 246.49 | J/molxK | 653.29 | Joback Method |
| dvisc | 0.0044123 | Paxs | 235.66 | Joback Method |
| dvisc | 0.0023483 | Paxs | 268.13 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0014322 | Paxs | 300.60 | Joback Method |
| dvisc | 0.0009619 | Paxs | 333.08 | Joback Method |
| dvisc | 0.0006934 | Paxs | 365.55 | Joback Method |
| dvisc | 0.0005273 | Paxs | 398.02 | Joback Method |
| dvisc | 0.0004178 | Paxs | 430.49 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R90868&Units=SI |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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<https://www.chemeo.com/cid/59-251-8/2H-Pyran-tetrahydro-2-6-dichloro-1.pdf>

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