# 2H-1,3-Oxazine, 2-(4-chlorophenyl)tetrahydro-

**Inchi:** InChI=1S/C10H12ClNO/c11-9-4-2-8(3-5-9)10-12-6-1-7-13-10/h2-5,10,12H,1,6-7H2
**InchiKey:** IUSGGJOQPVRUFH-UHFFFAOYSA-N
**Formula:** C10H12ClNO
**SMILES:** Clc1ccc(C2NCCCO2)cc1
**Mol. weight [g/mol]:** 197.66
**CAS:** 109086-75-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 150.21 | kJ/mol | Joback Method |
| hf | -80.28 | kJ/mol | Joback Method |
| hfus | 28.91 | kJ/mol | Joback Method |
| hvap | 56.87 | kJ/mol | Joback Method |
| log10ws | -2.92 | | Crippen Method |
| logp | 2.348 | | Crippen Method |
| mcvol | 145.230 | ml/mol | McGowan Method |
| pc | 3551.53 | kPa | Joback Method |
| tb | 592.34 | K | Joback Method |
| tc | 849.40 | K | Joback Method |
| tf | 410.30 | K | Joback Method |
| vc | 0.527 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 343.72 | J/mol×K | 592.34 | Joback Method |
| cpg | 360.72 | J/mol×K | 635.18 | Joback Method |
| cpg | 376.44 | J/mol×K | 678.03 | Joback Method |
| cpg | 390.93 | J/mol×K | 720.87 | Joback Method |
| cpg | 404.21 | J/mol×K | 763.71 | Joback Method |
| cpg | 416.34 | J/mol×K | 806.55 | Joback Method |
| cpg | 427.35 | J/mol×K | 849.40 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C109086751&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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 |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |