# trans-Wiskey lactone

**Inchi:** InChI=1S/C9H16O2/c1-3-4-5-8-7(2)6-9(10)11-8/h7-8H,3-6H2,1-2H3/t7-,8+/m1/s1
**InchiKey:** WNVCMFHPRIBNCW-SFYZADRCSA-N
**Formula:** C9H16O2
**SMILES:** CCCCC1OC(=O)CC1C
**Mol. weight [g/mol]:** 156.22

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -154.97 | kJ/mol | Joback Method |
| hf | -458.65 | kJ/mol | Joback Method |
| hfus | 21.56 | kJ/mol | Joback Method |
| hvap | 44.33 | kJ/mol | Joback Method |
| log10ws | -2.22 | | Crippen Method |
| logp | 2.128 | | Crippen Method |
| mcvol | 134.250 | ml/mol | McGowan Method |
| pc | 2744.03 | kPa | Joback Method |
| rinpol | 1258.00 | | NIST Webbook |
| ripol | 1861.00 | | NIST Webbook |
| tb | 510.70 | K | Joback Method |
| tc | 718.10 | K | Joback Method |
| tf | 292.64 | K | Joback Method |
| vc | 0.507 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 323.83 | J/mol×K | 510.70 | Joback Method |
| cpg | 340.60 | J/mol×K | 545.27 | Joback Method |
| cpg | 356.64 | J/mol×K | 579.83 | Joback Method |
| cpg | 371.95 | J/mol×K | 614.40 | Joback Method |
| cpg | 386.53 | J/mol×K | 648.97 | Joback Method |
| cpg | 400.37 | J/mol×K | 683.53 | Joback Method |
| cpg | 413.48 | J/mol×K | 718.10 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R586000&Units=SI |

# 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 |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |