# 2H-Pyran-3(4H)-one, 6-ethenyldihydro-2,2,6-trimethyl-

**Other names:** 2H-Pyran-3(4H)-one, dihydro-2,2,6-trimethyl-6-vinyl-
2,2,6-Trimethyl-3-keto-6-vinyltetrahydropyran
6-Ethenyldihydro-2,2,6-trimethyl-2H-pyran-3(4H)-one

**Inchi:** InChI=1S/C10H16O2/c1-5-10(4)7-6-8(11)9(2,3)12-10/h5H,1,6-7H2,2-4H3

**InchiKey:** ATQPZCOAQSYTPR-UHFFFAOYSA-N

**Formula:** C10H16O2

**SMILES:** C=CC1(C)CCC(=O)C(C)(C)O1

**Mol. weight [g/mol]:** 168.23

**CAS:** 33933-72-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -81.79 | kJ/mol | Joback Method |
| hf | -329.54 | kJ/mol | Joback Method |
| hfus | 8.17 | kJ/mol | Joback Method |
| hvap | 43.76 | kJ/mol | Joback Method |
| log10ws | -2.35 | | Crippen Method |
| logp | 2.089 | | Crippen Method |
| mcvol | 144.040 | ml/mol | McGowan Method |
| pc | 2928.17 | kPa | Joback Method |
| rinpol | 1106.00 | | NIST Webbook |
| rinpol | 1107.00 | | NIST Webbook |
| rinpol | 1107.00 | | NIST Webbook |
| rinpol | 1109.00 | | NIST Webbook |
| rinpol | 1109.00 | | NIST Webbook |
| rinpol | 1109.00 | | NIST Webbook |
| tb | 535.01 | K | Joback Method |
| tc | 770.10 | K | Joback Method |
| tf | 346.43 | K | Joback Method |
| vc | 0.532 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|

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|---|---|---|---|---|
| cpg | 351.47 | J/mol×K | 535.01 | Joback Method |
| cpg | 369.18 | J/mol×K | 574.19 | Joback Method |
| cpg | 385.73 | J/mol×K | 613.37 | Joback Method |
| cpg | 401.35 | J/mol×K | 652.56 | Joback Method |
| cpg | 416.23 | J/mol×K | 691.74 | Joback Method |
| cpg | 430.58 | J/mol×K | 730.92 | Joback Method |
| cpg | 444.63 | J/mol×K | 770.10 | 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=C33933721&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |