# Cyclohexanone, 5-methyl-2-(1-methylethenyl)-, trans-

**Other names:** p-Menth-8-en-3-one, trans-
trans-Isopulegone
Isopulegon
Isopulegone
trans-5-methyl-2-(1-methylvinyl)cyclohexan-1-one

**Inchi:** InChI=1S/C10H16O/c1-7(2)9-5-4-8(3)6-10(9)11/h8-9H,1,4-6H2,2-3H3/t8-,9+/m1/s1

**InchiKey:** RMIANEGNSBUGDJ-BDAKNGLRSA-N

**Formula:** C10H16O

**SMILES:** C=C(C)C1CCC(C)CC1=O

**Mol. weight [g/mol]:** 152.23

**CAS:** 29606-79-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 6.76 | kJ/mol | Joback Method |
| hf | -237.81 | kJ/mol | Joback Method |
| hfus | 11.48 | kJ/mol | Joback Method |
| hvap | 41.63 | kJ/mol | Joback Method |
| log10ws | -2.55 | | Crippen Method |
| logp | 2.568 | | Crippen Method |
| mcvol | 138.170 | ml/mol | McGowan Method |
| pc | 2701.41 | kPa | Joback Method |
| rinpol | 1159.00 | | NIST Webbook |
| rinpol | 1160.00 | | NIST Webbook |
| rinpol | 1199.00 | | NIST Webbook |
| rinpol | 1155.00 | | NIST Webbook |
| rinpol | 1152.00 | | NIST Webbook |
| rinpol | 1155.00 | | NIST Webbook |
| rinpol | 1155.00 | | NIST Webbook |
| rinpol | 1175.00 | | NIST Webbook |
| rinpol | 1175.00 | | NIST Webbook |
| rinpol | 1208.00 | | NIST Webbook |
| rinpol | 1192.00 | | NIST Webbook |
| rinpol | 1157.00 | | NIST Webbook |
| rinpol | 1188.00 | | NIST Webbook |
| rinpol | 1193.00 | | NIST Webbook |
| rinpol | 1177.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 1167.00 | | NIST Webbook |
| ripol | 1597.00 | | NIST Webbook |
| ripol | 1598.00 | | NIST Webbook |
| ripol | 1592.00 | | NIST Webbook |
| ripol | 1598.00 | | NIST Webbook |
| ripol | 1597.00 | | NIST Webbook |
| ripol | 1597.00 | | NIST Webbook |
| ripol | 1582.00 | | NIST Webbook |
| ripol | 1592.00 | | NIST Webbook |
| tb | 507.46 | K | Joback Method |
| tc | 729.79 | K | Joback Method |
| tf | 258.10 | K | Joback Method |
| vc | 0.516 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 320.01 | J/mol×K | 507.46 | Joback Method |
| cpg | 339.03 | J/mol×K | 544.51 | Joback Method |
| cpg | 357.13 | J/mol×K | 581.57 | Joback Method |
| cpg | 374.31 | J/mol×K | 618.62 | Joback Method |
| cpg | 390.57 | J/mol×K | 655.68 | Joback Method |
| cpg | 405.90 | J/mol×K | 692.73 | Joback Method |
| cpg | 420.31 | J/mol×K | 729.79 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C29606799&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 |
| **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 |