# Isocyclocitral

**Other names:** 3-Cyclohexene-1-carboxaldehyde, 2,4,6-trimethyl-, and 3,5,6-trimethyl-3-cyclohexene-1-carboxaldehyde
1-Formyl-3,5,6-trimethyl-3-cyclohexene and 1-formyl-2,4,6-trimethyl-3-cyclohexene

**Inchi:** InChI=1S/C10H16O/c1-7-4-8(2)9(3)10(5-7)6-11/h4,6,8-10H,5H2,1-3H3

**InchiKey:** DEMWVPUIZCCHPT-UHFFFAOYSA-N

**Formula:** C10H16O

**SMILES:** CC1=CC(C)C(C)C(C=O)C1

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

**CAS:** 1335-66-6

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -36.84 | kJ/mol | Joback Method |
| hf | -275.36 | kJ/mol | Joback Method |
| hfus | 18.75 | kJ/mol | Joback Method |
| hvap | 45.34 | kJ/mol | Joback Method |
| log10ws | -2.31 | | Crippen Method |
| logp | 2.424 | | Crippen Method |
| mcvol | 138.170 | ml/mol | McGowan Method |
| pc | 2646.11 | kPa | Joback Method |
| rinpol | 1117.00 | | NIST Webbook |
| rinpol | 1119.90 | | NIST Webbook |
| ripol | 1515.00 | | NIST Webbook |
| tb | 491.21 | K | Joback Method |
| tc | 695.98 | K | Joback Method |
| tf | 256.64 | K | Joback Method |
| vc | 0.529 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 313.91 | J/mol×K | 491.21 | Joback Method |
| cpg | 331.02 | J/mol×K | 525.34 | Joback Method |
| cpg | 347.33 | J/mol×K | 559.47 | Joback Method |
| cpg | 362.84 | J/mol×K | 593.59 | Joback Method |

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|---|---|---|---|---|
| cpg | 377.58 | J/mol×K | 627.72 | Joback Method |
| cpg | 391.54 | J/mol×K | 661.85 | Joback Method |
| cpg | 404.74 | J/mol×K | 695.98 | Joback Method |
| dvisc | 0.0018898 | Pa×s | 256.64 | Joback Method |
| dvisc | 0.0011726 | Pa×s | 295.74 | Joback Method |
| dvisc | 0.0008133 | Pa×s | 334.83 | Joback Method |
| dvisc | 0.0006090 | Pa×s | 373.92 | Joback Method |
| dvisc | 0.0004817 | Pa×s | 413.02 | Joback Method |
| dvisc | 0.0003967 | Pa×s | 452.12 | Joback Method |
| dvisc | 0.0003370 | Pa×s | 491.21 | 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=C1335666&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
**ripol:** Polar retention indices
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume