# Cyclohexene-1-acetaldehyde, 2,6,6-trimethyl

**Inchi:** InChI=1S/C10H18O/c1-8-5-4-6-10(2,3)9(8)7-11/h7-9H,4-6H2,1-3H3
**InchiKey:** MPLGIGIOVUTMJA-UHFFFAOYSA-N
**Formula:** C10H18O
**SMILES:** CC1CCCC(C)(C)C1C=O
**Mol. weight [g/mol]:** 154.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -62.66 | kJ/mol | Joback Method |
| hf | -306.43 | kJ/mol | Joback Method |
| hfus | 11.62 | kJ/mol | Joback Method |
| hvap | 43.23 | kJ/mol | Joback Method |
| log10ws | -2.46 | | Crippen Method |
| logp | 2.648 | | Crippen Method |
| mcvol | 142.470 | ml/mol | McGowan Method |
| pc | 2712.67 | kPa | Joback Method |
| rinpol | 1238.00 | | NIST Webbook |
| tb | 487.31 | K | Joback Method |
| tc | 697.48 | K | Joback Method |
| tf | 267.26 | K | Joback Method |
| vc | 0.541 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 329.83 | J/mol×K | 487.31 | Joback Method |
| cpg | 348.62 | J/mol×K | 522.34 | Joback Method |
| cpg | 366.29 | J/mol×K | 557.37 | Joback Method |
| cpg | 382.94 | J/mol×K | 592.39 | Joback Method |
| cpg | 398.65 | J/mol×K | 627.42 | Joback Method |
| cpg | 413.51 | J/mol×K | 662.45 | Joback Method |
| cpg | 427.62 | J/mol×K | 697.48 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R199656&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

Latest version available from:
https://www.chemeo.com/cid/76-491-3/Cyclohexene-1-acetaldehyde-2-6-6-trimethyl.pdf
Generated by Cheméo on 2024-10-12 09:12:26.624312825 +0000 UTC m=+3305209.261282073.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.