# 3-Cyclohexene-1-carboxaldehyde, 4-(4-methyl-3-pentenyl)-

**Other names:** Myrac aldehyde 2
4-(4-Methyl-3-pentenyl)-3-cyclohexene-1-carbaldehyde
3-Cyclohexene-1-carboxaldehyde, 4-(4-methyl-3-penten-1-yl)-
4-(4-Methyl-3-pentenyl)cyclohex-3-ene-1-carbaldehyde
1-Formyl-4-isohexenyl-4-cyclohexene
p-Myrac aldehyde
Myrac aldehyde
Emfetal

**Inchi:** InChI=1S/C13H20O/c1-11(2)4-3-5-12-6-8-13(10-14)9-7-12/h4,6,10,13H,3,5,7-9H2,1-2H3

**InchiKey:** MQBIZQLCHSZBOI-UHFFFAOYSA-N

**Formula:** C13H20O

**SMILES:** CC(C)=CCCC1=CCC(C=O)CC1

**Mol. weight [g/mol]:** 192.30

**CAS:** 37677-14-8

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 75.51 | kJ/mol | Joback Method |
| hf | -189.17 | kJ/mol | Joback Method |
| hfus | 23.28 | kJ/mol | Joback Method |
| hvap | 52.67 | kJ/mol | Joback Method |
| log10ws | -3.90 | | Crippen Method |
| logp | 3.658 | | Crippen Method |
| mcvol | 176.140 | ml/mol | McGowan Method |
| pc | 2248.26 | kPa | Joback Method |
| rinpol | 1497.30 | | NIST Webbook |
| rinpol | 1509.00 | | NIST Webbook |
| rinpol | 1497.30 | | NIST Webbook |
| rinpol | 1509.00 | | NIST Webbook |
| ripol | 1978.00 | | NIST Webbook |
| ripol | 1978.00 | | NIST Webbook |
| tb | 573.23 | K | Joback Method |
| tc | 781.91 | K | Joback Method |
| tf | 279.89 | K | Joback Method |
| vc | 0.680 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 438.64 | J/mol×K | 573.23 | Joback Method |
| cpg | 456.92 | J/mol×K | 608.01 | Joback Method |
| cpg | 474.14 | J/mol×K | 642.79 | Joback Method |
| cpg | 490.35 | J/mol×K | 677.57 | Joback Method |
| cpg | 505.60 | J/mol×K | 712.35 | Joback Method |
| cpg | 519.93 | J/mol×K | 747.13 | Joback Method |
| cpg | 533.39 | J/mol×K | 781.91 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C37677148&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

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|---|---|
| **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 |