# 4-(2,2-Dimethyl-6-methylenecyclohexyl)butanal

**Inchi:** InChI=1S/C13H22O/c1-11-7-6-9-13(2,3)12(11)8-4-5-10-14/h10,12H,1,4-9H2,2-3H3
**InchiKey:** LEXVMOJLXLEPJE-UHFFFAOYSA-N
**Formula:** C13H22O
**SMILES:** C=C1CCCC(C)(C)C1CCCC=O
**Mol. weight [g/mol]:** 194.31
**CAS:** 95452-13-4

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 23.39 | kJ/mol | Joback Method |
| hf | -263.77 | kJ/mol | Joback Method |
| hfus | 17.16 | kJ/mol | Joback Method |
| hvap | 50.38 | kJ/mol | Joback Method |
| log10ws | -3.81 | | Crippen Method |
| logp | 3.738 | | Crippen Method |
| mcvol | 180.440 | ml/mol | McGowan Method |
| pc | 2151.31 | kPa | Joback Method |
| rinpol | 1703.00 | | NIST Webbook |
| tb | 559.78 | K | Joback Method |
| tc | 762.61 | K | Joback Method |
| tf | 318.99 | K | Joback Method |
| vc | 0.695 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 456.24 | J/mol×K | 559.78 | Joback Method |
| cpg | 475.07 | J/mol×K | 593.58 | Joback Method |
| cpg | 492.88 | J/mol×K | 627.39 | Joback Method |
| cpg | 509.76 | J/mol×K | 661.19 | Joback Method |
| cpg | 525.81 | J/mol×K | 695.00 | Joback Method |
| cpg | 541.11 | J/mol×K | 728.80 | Joback Method |
| cpg | 555.76 | J/mol×K | 762.61 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C95452134&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 |