# 4-methyl-2-phenyl-2-hexenal

**Inchi:** InChI=1S/C13H16O/c1-3-11(2)9-13(10-14)12-7-5-4-6-8-12/h4-11H,3H2,1-2H3/b13-9-
**InchiKey:** IOIWDGZFMUCYJR-LCYFTJDESA-N
**Formula:** C13H16O
**SMILES:** CCC(C)C=C(C=O)c1ccccc1
**Mol. weight [g/mol]:** 188.27

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 140.70 | kJ/mol | Joback Method |
| hf | -58.55 | kJ/mol | Joback Method |
| hfus | 21.13 | kJ/mol | Joback Method |
| hvap | 53.18 | kJ/mol | Joback Method |
| log10ws | -3.43 | | Crippen Method |
| logp | 3.315 | | Crippen Method |
| mcvol | 167.540 | ml/mol | McGowan Method |
| pc | 2510.03 | kPa | Joback Method |
| ripol | 2000.00 | | NIST Webbook |
| ripol | 2000.00 | | NIST Webbook |
| tb | 575.78 | K | Joback Method |
| tc | 792.99 | K | Joback Method |
| tf | 270.65 | K | Joback Method |
| vc | 0.647 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 398.02 | J/mol×K | 575.78 | Joback Method |
| cpg | 414.02 | J/mol×K | 611.98 | Joback Method |
| cpg | 428.96 | J/mol×K | 648.18 | Joback Method |
| cpg | 442.92 | J/mol×K | 684.39 | Joback Method |
| cpg | 455.95 | J/mol×K | 720.59 | Joback Method |
| cpg | 468.11 | J/mol×K | 756.79 | Joback Method |
| cpg | 479.46 | J/mol×K | 792.99 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R308182&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 |

# 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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |