# Octanal, 2-(phenylmethylene)-

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|---|---|
| **Other names:** | Cinnamaldehyde, «alpha»-hexyl- |
| | «alpha»-n-Hexyl-«beta»-phenylacrolein |
| | «alpha»-Hexylcinnamaldehyde |
| | «alpha»-Hexylcinnamic aldehyde |
| | Hexyl cinnamic aldehyde |
| | 2-Hexyl-3-phenyl-2-propenal |
| | 2-Hexyl-3-phenyl-propenal |
| | n-Hexyl cinnamaldehyde |
| | 2-(Phenylmethylene)octanal |
| | 2-Hexylcinnamaldehyde |
| | NSC 406799 |
| | «alpha»-Hexylcinnamyl aldehyde |
| | Hexylcinnamaldehyde |
| **Inchi:** | InChI=1S/C15H20O/c1-2-3-4-6-11-15(13-16)12-14-9-7-5-8-10-14/h5,7-10,12-13H,2-4,6,1 |
| **InchiKey:** | GUUHFMWKWLOQMM-QINSGFPZSA-N |
| **Formula:** | C15H20O |
| **SMILES:** | CCCCCCC(C=O)=Cc1ccccc1 |
| **Mol. weight [g/mol]:** | 216.32 |
| **CAS:** | 101-86-0 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 159.98 | kJ/mol | Joback Method |
| hf | -94.55 | kJ/mol | Joback Method |
| hfus | 29.83 | kJ/mol | Joback Method |
| hvap | 58.02 | kJ/mol | Joback Method |
| log10ws | -4.51 | | Crippen Method |
| logp | 4.239 | | Crippen Method |
| mcvol | 195.720 | ml/mol | McGowan Method |
| pc | 2073.65 | kPa | Joback Method |
| rinpol | 1747.00 | | NIST Webbook |
| rinpol | 1764.00 | | NIST Webbook |
| rinpol | 1763.00 | | NIST Webbook |
| rinpol | 1764.00 | | NIST Webbook |
| rinpol | 1765.00 | | NIST Webbook |
| rinpol | 1750.00 | | NIST Webbook |
| rinpol | 1770.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 1746.00 | | NIST Webbook |
| rinpol | 1728.00 | | NIST Webbook |
| rinpol | 1727.00 | | NIST Webbook |
| rinpol | 1726.20 | | NIST Webbook |
| rinpol | 1746.00 | | NIST Webbook |
| rinpol | 1764.00 | | NIST Webbook |
| rinpol | 1770.00 | | NIST Webbook |
| rinpol | 1746.00 | | NIST Webbook |
| rinpol | 1743.00 | | NIST Webbook |
| rinpol | 1746.00 | | NIST Webbook |
| rinpol | 1726.20 | | NIST Webbook |
| rinpol | 1766.00 | | NIST Webbook |
| rinpol | 1728.00 | | NIST Webbook |
| ripol | 2309.00 | | NIST Webbook |
| tb | 621.98 | K | Joback Method |
| tc | 827.96 | K | Joback Method |
| tf | 308.19 | K | Joback Method |
| vc | 0.765 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 497.60 | J/mol×K | 621.98 | Joback Method |
| cpg | 514.24 | J/mol×K | 656.31 | Joback Method |
| cpg | 529.87 | J/mol×K | 690.64 | Joback Method |
| cpg | 544.54 | J/mol×K | 724.97 | Joback Method |
| cpg | 558.31 | J/mol×K | 759.30 | Joback Method |
| cpg | 571.25 | J/mol×K | 793.63 | Joback Method |
| cpg | 583.40 | J/mol×K | 827.96 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 448.20 | K | 2.00 | NIST Webbook |

# Sources

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|---|---|
| **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=C101860&Units=SI |

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

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