# «beta»-Sinensal

**Other names:** 2,6-dimethyl-10-methylenedodeca-2,6,11-trien-1-al
**Inchi:** InChI=1S/C15H22O/c1-5-13(2)8-6-9-14(3)10-7-11-15(4)12-16/h5,9,11-12H,1-2,6-8,10H2
**InchiKey:** NOPLRNXKHZRXHT-YFVJMOTDSA-N
**Formula:** C15H22O
**SMILES:** C=CC(=C)CCC=C(C)CCC=C(C)C=O
**Mol. weight [g/mol]:** 218.33
**CAS:** 60066-88-8

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 286.37 | kJ/mol | Joback Method |
| hf | 17.42 | kJ/mol | Joback Method |
| hfus | 30.81 | kJ/mol | Joback Method |
| hvap | 54.52 | kJ/mol | Joback Method |
| log10ws | -4.80 | | Crippen Method |
| logp | 4.381 | | Crippen Method |
| mcvol | 206.580 | ml/mol | McGowan Method |
| pc | 1763.93 | kPa | Joback Method |
| rinpol | 1707.00 | | NIST Webbook |
| rinpol | 1664.00 | | NIST Webbook |
| rinpol | 1706.00 | | NIST Webbook |
| rinpol | 1700.00 | | NIST Webbook |
| rinpol | 1673.00 | | NIST Webbook |
| rinpol | 1668.00 | | NIST Webbook |
| rinpol | 1695.00 | | NIST Webbook |
| rinpol | 1673.00 | | NIST Webbook |
| rinpol | 1673.00 | | NIST Webbook |
| rinpol | 1685.00 | | NIST Webbook |
| rinpol | 1671.00 | | NIST Webbook |
| rinpol | 1672.00 | | NIST Webbook |
| rinpol | 1671.00 | | NIST Webbook |
| rinpol | 1706.00 | | NIST Webbook |
| rinpol | 1694.00 | | NIST Webbook |
| rinpol | 1675.00 | | NIST Webbook |
| rinpol | 1659.00 | | NIST Webbook |
| rinpol | 1695.00 | | NIST Webbook |
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|---|---|---|
| rinpol | 1658.00 | NIST Webbook |
| rinpol | 1673.00 | NIST Webbook |
| rinpol | 1672.00 | NIST Webbook |
| rinpol | 1691.00 | NIST Webbook |
| rinpol | 1669.00 | NIST Webbook |
| rinpol | 1671.00 | NIST Webbook |
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| rinpol | 1671.00 | NIST Webbook |
| rinpol | 1671.00 | NIST Webbook |
| rinpol | 1671.00 | NIST Webbook |
| rinpol | 1697.00 | NIST Webbook |
| rinpol | 1700.00 | NIST Webbook |
| rinpol | 1697.00 | NIST Webbook |
| rinpol | 1702.50 | NIST Webbook |
| rinpol | 1661.00 | NIST Webbook |
| rinpol | 1658.00 | NIST Webbook |
| rinpol | 1671.00 | NIST Webbook |
| rinpol | 1677.00 | NIST Webbook |
| rinpol | 1664.00 | NIST Webbook |
| rinpol | 1693.00 | NIST Webbook |
| rinpol | 1694.00 | NIST Webbook |
| rinpol | 1702.50 | NIST Webbook |
| ripol | 2200.00 | NIST Webbook |
| ripol | 2249.00 | NIST Webbook |
| ripol | 2254.00 | NIST Webbook |
| ripol | 2242.00 | NIST Webbook |
| ripol | 2200.00 | NIST Webbook |
| ripol | 2249.00 | NIST Webbook |
| ripol | 2225.00 | NIST Webbook |
| ripol | 2244.00 | NIST Webbook |
| ripol | 2239.00 | NIST Webbook |
| ripol | 2225.00 | NIST Webbook |
| ripol | 2225.00 | NIST Webbook |
| ripol | 2189.00 | NIST Webbook |
| ripol | 2251.00 | NIST Webbook |
| ripol | 2251.00 | NIST Webbook |
| ripol | 2228.00 | NIST Webbook |
| ripol | 2249.00 | NIST Webbook |
| ripol | 2249.00 | NIST Webbook |
| ripol | 2238.00 | NIST Webbook |
| ripol | 2237.00 | NIST Webbook |
| ripol | 2237.00 | NIST Webbook |

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|---|---|---|---|
| ripol | 2225.00 | | NIST Webbook |
| ripol | 2237.00 | | NIST Webbook |
| ripol | 2200.00 | | NIST Webbook |
| ripol | 2209.00 | | NIST Webbook |
| ripol | 2251.00 | | NIST Webbook |
| ripol | 2238.00 | | NIST Webbook |
| ripol | 2242.00 | | NIST Webbook |
| ripol | 2239.00 | | NIST Webbook |
| ripol | 2228.00 | | NIST Webbook |
| ripol | 2203.00 | | NIST Webbook |
| ripol | 2250.00 | | NIST Webbook |
| ripol | 2250.00 | | NIST Webbook |
| tb | 592.58 | K | Joback Method |
| tc | 782.72 | K | Joback Method |
| tf | 245.25 | K | Joback Method |
| vc | 0.818 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 508.03 | J/mol×K | 592.58 | Joback Method |
| cpg | 524.29 | J/mol×K | 624.27 | Joback Method |
| cpg | 539.65 | J/mol×K | 655.96 | Joback Method |
| cpg | 554.19 | J/mol×K | 687.65 | Joback Method |
| cpg | 567.94 | J/mol×K | 719.34 | Joback Method |
| cpg | 580.98 | J/mol×K | 751.03 | Joback Method |
| cpg | 593.36 | J/mol×K | 782.72 | Joback Method |

# Sources

**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=C60066888&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 |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |