# 2-Dodecenal, (E)-

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|---|---|
| **Other names:** | (2E)-2-Dodecenal |
| | (E)-2-Dodecen-1-al |
| | (E)-2-Dodecenal |
| | (E)-Dodec-2-enal |
| | (E)-dodec-2-en-1-al |
| | 2(E)-Dodecenal |
| | trans-2-Dodecenal |
| | trans-Dodec-2-enal |
| **Inchi:** | InChI=1S/C12H22O/c1-2-3-4-5-6-7-8-9-10-11-12-13/h10-12H,2-9H2,1H3/b11-10+ |
| **InchiKey:** | SSNZFFBDIMUILS-ZHACJKMWSA-N |
| **Formula:** | C12H22O |
| **SMILES:** | CCCCCCCCCC=CC=O |
| **Mol. weight [g/mol]:** | 182.30 |
| **CAS:** | 20407-84-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 30.86 | kJ/mol | Joback Method |
| hf | -259.37 | kJ/mol | Joback Method |
| hfus | 29.33 | kJ/mol | Joback Method |
| hvap | 72.60 | kJ/mol | NIST Webbook |
| log10ws | -3.98 | | Crippen Method |
| logp | 3.882 | | Crippen Method |
| mcvol | 177.210 | ml/mol | McGowan Method |
| pc | 1985.89 | kPa | Joback Method |
| rinpol | 1442.00 | | NIST Webbook |
| rinpol | 1462.00 | | NIST Webbook |
| rinpol | 1466.00 | | NIST Webbook |
| rinpol | 1452.00 | | NIST Webbook |
| rinpol | 1458.00 | | NIST Webbook |
| rinpol | 1448.00 | | NIST Webbook |
| rinpol | 1444.00 | | NIST Webbook |
| rinpol | 1445.00 | | NIST Webbook |
| rinpol | 1467.50 | | NIST Webbook |
| rinpol | 1468.00 | | NIST Webbook |
| rinpol | 1460.00 | | NIST Webbook |
| rinpol | 1471.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 1444.00 | | NIST Webbook |
| rinpol | 1445.00 | | NIST Webbook |
| rinpol | 1445.00 | | NIST Webbook |
| rinpol | 1482.00 | | NIST Webbook |
| rinpol | 1466.00 | | NIST Webbook |
| rinpol | 1468.00 | | NIST Webbook |
| rinpol | 1444.00 | | NIST Webbook |
| rinpol | 1467.50 | | NIST Webbook |
| rinpol | 1468.00 | | NIST Webbook |
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| rinpol | 1471.00 | | NIST Webbook |
| rinpol | 1462.00 | | NIST Webbook |
| rinpol | 1444.00 | | NIST Webbook |
| rinpol | 1439.00 | | NIST Webbook |
| rinpol | 1464.00 | | NIST Webbook |
| rinpol | 1442.00 | | NIST Webbook |
| rinpol | 1472.00 | | NIST Webbook |
| rinpol | 1445.00 | | NIST Webbook |
| rinpol | 1462.00 | | NIST Webbook |
| ripol | 1849.00 | | NIST Webbook |
| ripol | 1860.00 | | NIST Webbook |
| ripol | 1835.00 | | NIST Webbook |
| ripol | 1866.00 | | NIST Webbook |
| ripol | 1872.00 | | NIST Webbook |
| ripol | 1851.00 | | NIST Webbook |
| ripol | 1867.00 | | NIST Webbook |
| ripol | 1844.00 | | NIST Webbook |
| ripol | 1871.00 | | NIST Webbook |
| ripol | 1889.00 | | NIST Webbook |
| ripol | 1889.00 | | NIST Webbook |
| ripol | 1901.00 | | NIST Webbook |
| ripol | 1865.00 | | NIST Webbook |
| ripol | 1867.00 | | NIST Webbook |
| ripol | 1867.00 | | NIST Webbook |
| ripol | 1887.00 | | NIST Webbook |
| ripol | 1844.00 | | NIST Webbook |
| ripol | 1838.00 | | NIST Webbook |
| ripol | 1871.00 | | NIST Webbook |
| ripol | 1867.00 | | NIST Webbook |
| ripol | 1835.00 | | NIST Webbook |
| tb | 526.78 | K | Joback Method |
| tc | 700.00 | K | Joback Method |
| tf | 261.92 | K | Joback Method |
| vc | 0.705 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 418.84 | J/mol×K | 526.78 | Joback Method |
| cpg | 488.73 | J/mol×K | 671.13 | Joback Method |
| cpg | 476.02 | J/mol×K | 642.26 | Joback Method |
| cpg | 462.70 | J/mol×K | 613.39 | Joback Method |
| cpg | 448.75 | J/mol×K | 584.52 | Joback Method |
| cpg | 434.14 | J/mol×K | 555.65 | Joback Method |
| cpg | 500.86 | J/mol×K | 700.00 | Joback Method |
| dvisc | 0.0002140 | Pa×s | 526.78 | Joback Method |
| dvisc | 0.0002830 | Pa×s | 482.64 | Joback Method |
| dvisc | 0.0003959 | Pa×s | 438.49 | Joback Method |
| dvisc | 0.0005970 | Pa×s | 394.35 | Joback Method |
| dvisc | 0.0009985 | Pa×s | 350.21 | Joback Method |
| dvisc | 0.0019373 | Pa×s | 306.06 | Joback Method |
| dvisc | 0.0046993 | Pa×s | 261.92 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.42287e+01 |
| Coeff. B | -4.33600e+03 |
| Coeff. C | -8.76980e+01 |
| Temperature range (K), min. | 398.72 |
| Temperature range (K), max. | 573.95 |

# 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

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C20407845&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |
| **pvap:** | Vapor 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 |