# 2-Undecenal

| | |
|---|---|
| **Other names:** | 2-Undecen-1-al |
| | Undec-2-enal |
| **Inchi:** | InChI=1S/C11H20O/c1-2-3-4-5-6-7-8-9-10-11-12/h9-11H,2-8H2,1H3/b10-9+ |
| **InchiKey:** | PANBRUWVURLWGY-MDZDMXLPSA-N |
| **Formula:** | C11H20O |
| **SMILES:** | CCCCCCCCC=CC=O |
| **Mol. weight [g/mol]:** | 168.28 |
| **CAS:** | 2463-77-6 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 22.44 | kJ/mol | Joback Method |
| hf | -238.73 | kJ/mol | Joback Method |
| hfus | 26.74 | kJ/mol | Joback Method |
| hvap | 46.76 | kJ/mol | Joback Method |
| log10ws | -3.56 | | Crippen Method |
| logp | 3.492 | | Crippen Method |
| mcvol | 163.120 | ml/mol | McGowan Method |
| pc | 2167.36 | kPa | Joback Method |
| rinpol | 1373.00 | | NIST Webbook |
| rinpol | 1346.00 | | NIST Webbook |
| rinpol | 1371.00 | | NIST Webbook |
| rinpol | 1335.00 | | NIST Webbook |
| rinpol | 1359.00 | | NIST Webbook |
| rinpol | 1360.00 | | NIST Webbook |
| rinpol | 1341.00 | | NIST Webbook |
| rinpol | 1350.00 | | NIST Webbook |
| rinpol | 1339.00 | | NIST Webbook |
| rinpol | 1346.00 | | NIST Webbook |
| rinpol | 1376.00 | | NIST Webbook |
| rinpol | 1376.00 | | NIST Webbook |
| rinpol | 1350.00 | | NIST Webbook |
| rinpol | 1350.00 | | NIST Webbook |
| rinpol | 1370.00 | | NIST Webbook |
| rinpol | 1368.00 | | NIST Webbook |
| rinpol | 1350.00 | | NIST Webbook |
| rinpol | 1346.00 | | NIST Webbook |

| | | | |
|---|---|---|---|
| rinpol | 1342.00 | | NIST Webbook |
| rinpol | 1340.00 | | NIST Webbook |
| rinpol | 1342.00 | | NIST Webbook |
| rinpol | 1342.00 | | NIST Webbook |
| rinpol | 1353.00 | | NIST Webbook |
| rinpol | 1363.00 | | NIST Webbook |
| rinpol | 1341.00 | | NIST Webbook |
| rinpol | 1344.00 | | NIST Webbook |
| rinpol | 1375.00 | | NIST Webbook |
| rinpol | 1368.00 | | NIST Webbook |
| rinpol | 1344.00 | | NIST Webbook |
| rinpol | 1367.00 | | NIST Webbook |
| rinpol | 1366.00 | | NIST Webbook |
| rinpol | 1366.00 | | NIST Webbook |
| rinpol | 1359.00 | | NIST Webbook |
| rinpol | 1369.00 | | NIST Webbook |
| rinpol | 1339.00 | | NIST Webbook |
| rinpol | 1341.00 | | NIST Webbook |
| ripol | 1740.00 | | NIST Webbook |
| ripol | 1736.00 | | NIST Webbook |
| ripol | 1740.00 | | NIST Webbook |
| ripol | 1747.00 | | NIST Webbook |
| ripol | 1736.00 | | NIST Webbook |
| ripol | 1755.00 | | NIST Webbook |
| ripol | 1755.00 | | NIST Webbook |
| ripol | 1755.00 | | NIST Webbook |
| ripol | 1755.00 | | NIST Webbook |
| tb | 503.90 | K | Joback Method |
| tc | 678.56 | K | Joback Method |
| tf | 250.65 | K | Joback Method |
| vc | 0.648 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 371.55 | J/mol×K | 503.90 | Joback Method |
| cpg | 438.14 | J/mol×K | 649.45 | Joback Method |
| cpg | 426.04 | J/mol×K | 620.34 | Joback Method |
| cpg | 413.35 | J/mol×K | 591.23 | Joback Method |
| cpg | 400.06 | J/mol×K | 562.12 | Joback Method |
| cpg | 386.13 | J/mol×K | 533.01 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 449.68 | J/mol×K | 678.56 | Joback Method |
| dvisc | 0.0002297 | Pa×s | 503.90 | Joback Method |
| dvisc | 0.0003024 | Pa×s | 461.69 | Joback Method |
| dvisc | 0.0004207 | Pa×s | 419.48 | Joback Method |
| dvisc | 0.0006302 | Pa×s | 377.27 | Joback Method |
| dvisc | 0.0010451 | Pa×s | 335.07 | Joback Method |
| dvisc | 0.0020053 | Pa×s | 292.86 | Joback Method |
| dvisc | 0.0047920 | Pa×s | 250.65 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.42916e+01 |
| Coeff. B | -4.23130e+03 |
| Coeff. C | -8.29720e+01 |
| Temperature range (K), min. | 385.12 |
| Temperature range (K), max. | 554.15 |

# Sources

| | |
|---|---|
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **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=C2463776&Units=SI |

# 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 |

Latest version available from:

https://www.chemeo.com/cid/21-974-7/2-Undecenal.pdf

Generated by Cheméo on 2024-10-12 08:59:00.969813869 +0000 UTC m=+3304403.606783118.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.