# 2-Octanol

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|---|---|
| **Other names:** | 1-Methyl-1-heptanol |
| | 1-Methylheptanol |
| | 1-Methylheptyl alcohol |
| | 2-Hydroxy-n-octane |
| | 2-Hydroxyoctane |
| | 2-Octanol, (.+/-.)- |
| | 2-Octyl alcohol |
| | Capryl alcohol |
| | Hexylmethylcarbinol |
| | Methylhexylcarbinol |
| | NSC 14759 |
| | Octan-2-ol |
| | Octanol-2 |
| | methylheptanol |
| | n-Octan-2-ol |
| | s-Octyl alcohol |
| | sec-Caprylic alcohol |
| | sec-Octyl alcohol |
| | «beta»-Octyl alcohol |
| | Â«betaÂ»-Octyl alcohol |
| **Inchi:** | InChI=1S/C8H18O/c1-3-4-5-6-7-8(2)9/h8-9H,3-7H2,1-2H3 |
| **InchiKey:** | SJWFXCIHNDVPSH-UHFFFAOYSA-N |
| **Formula:** | C8H18O |
| **SMILES:** | CCCCCCC(C)O |
| **Mol. weight [g/mol]:** | 130.23 |
| **CAS:** | 123-96-6 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -122.78 | kJ/mol | Joback Method |
| hf | -365.96 | kJ/mol | Joback Method |
| hfus | 17.04 | kJ/mol | Joback Method |
| hvap | 67.90 ± 0.30 | kJ/mol | NIST Webbook |
| log10ws | -2.55 | | Crippen Method |
| logp | 2.338 | | Crippen Method |
| mcvol | 129.450 | ml/mol | McGowan Method |
| pc | 2750.00 ± 50.00 | kPa | NIST Webbook |

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|---|---|---|---|
| pc | 2727.00 ± 0.02 | kPa | NIST Webbook |
| pc | 2900.00 ± 200.00 | kPa | NIST Webbook |
| pc | 2780.00 ± 50.00 | kPa | NIST Webbook |
| pc | 2727.00 ± 20.00 | kPa | NIST Webbook |
| rhoc | 251.34 ± 6.51 | kg/m3 | NIST Webbook |
| rhoc | 251.34 ± 6.51 | kg/m3 | NIST Webbook |
| rinpol | 988.00 | | NIST Webbook |
| rinpol | 997.00 | | NIST Webbook |
| rinpol | 995.00 | | NIST Webbook |
| rinpol | 1002.00 | | NIST Webbook |
| rinpol | 1002.00 | | NIST Webbook |
| rinpol | 1002.00 | | NIST Webbook |
| rinpol | 1004.00 | | NIST Webbook |
| rinpol | 998.00 | | NIST Webbook |
| rinpol | 990.00 | | NIST Webbook |
| rinpol | 1002.00 | | NIST Webbook |
| rinpol | 1010.00 | | NIST Webbook |
| rinpol | 995.00 | | NIST Webbook |
| rinpol | 984.00 | | NIST Webbook |
| rinpol | 990.00 | | NIST Webbook |
| rinpol | 992.00 | | NIST Webbook |
| rinpol | 987.00 | | NIST Webbook |
| rinpol | 988.00 | | NIST Webbook |
| rinpol | 983.00 | | NIST Webbook |
| rinpol | 982.00 | | NIST Webbook |
| rinpol | 985.00 | | NIST Webbook |
| rinpol | 994.00 | | NIST Webbook |
| rinpol | 1002.00 | | NIST Webbook |
| rinpol | 990.00 | | NIST Webbook |
| rinpol | 990.00 | | NIST Webbook |
| rinpol | 1013.00 | | NIST Webbook |
| rinpol | 1011.00 | | NIST Webbook |
| rinpol | 1003.00 | | NIST Webbook |
| rinpol | 982.00 | | NIST Webbook |
| rinpol | 1004.00 | | NIST Webbook |
| rinpol | 983.00 | | NIST Webbook |
| rinpol | 1018.00 | | NIST Webbook |
| rinpol | 984.00 | | NIST Webbook |
| rinpol | 984.00 | | NIST Webbook |
| rinpol | 161.85 | | NIST Webbook |
| rinpol | 995.00 | | NIST Webbook |
| rinpol | 998.00 | | NIST Webbook |
| rinpol | 984.00 | | NIST Webbook |
| rinpol | 983.00 | | NIST Webbook |

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|---|---|---|
| rinpol | 161.85 | NIST Webbook |
| rinpol | 1012.00 | NIST Webbook |
| rinpol | 1014.00 | NIST Webbook |
| rinpol | 998.00 | NIST Webbook |
| rinpol | 1012.00 | NIST Webbook |
| rinpol | 1011.00 | NIST Webbook |
| rinpol | 997.00 | NIST Webbook |
| rinpol | 990.00 | NIST Webbook |
| rinpol | 990.00 | NIST Webbook |
| rinpol | 979.00 | NIST Webbook |
| rinpol | 966.00 | NIST Webbook |
| rinpol | 976.70 | NIST Webbook |
| rinpol | 977.00 | NIST Webbook |
| rinpol | 1009.00 | NIST Webbook |
| rinpol | 962.00 | NIST Webbook |
| ripol | 1412.00 | NIST Webbook |
| ripol | 1421.00 | NIST Webbook |
| ripol | 1421.00 | NIST Webbook |
| ripol | 1430.00 | NIST Webbook |
| ripol | 1409.00 | NIST Webbook |
| ripol | 1412.00 | NIST Webbook |
| ripol | 1399.00 | NIST Webbook |
| ripol | 1418.00 | NIST Webbook |
| ripol | 1421.00 | NIST Webbook |
| ripol | 1380.00 | NIST Webbook |
| ripol | 1385.00 | NIST Webbook |
| ripol | 1396.00 | NIST Webbook |
| ripol | 1421.00 | NIST Webbook |
| ripol | 1430.00 | NIST Webbook |
| ripol | 1398.00 | NIST Webbook |
| ripol | 1398.00 | NIST Webbook |
| ripol | 1394.00 | NIST Webbook |
| ripol | 1398.00 | NIST Webbook |
| ripol | 1418.00 | NIST Webbook |
| ripol | 1422.00 | NIST Webbook |
| ripol | 1416.00 | NIST Webbook |
| ripol | 1420.00 | NIST Webbook |
| ripol | 1430.00 | NIST Webbook |
| ripol | 1423.00 | NIST Webbook |
| ripol | 1422.00 | NIST Webbook |
| ripol | 1405.00 | NIST Webbook |
| ripol | 1384.00 | NIST Webbook |
| ripol | 1411.00 | NIST Webbook |
| ripol | 1385.00 | NIST Webbook |

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|---|---|---|---|
| ripol | 1384.00 | | NIST Webbook |
| ripol | 1385.00 | | NIST Webbook |
| ripol | 1390.00 | | NIST Webbook |
| tb | 474.18 | K | Joback Method |
| tc | 629.70 ± 0.30 | K | NIST Webbook |
| tc | 629.40 | K | NIST Webbook |
| tc | 629.00 ± 0.60 | K | NIST Webbook |
| tc | 629.00 ± 0.60 | K | NIST Webbook |
| tc | 638.00 ± 3.00 | K | NIST Webbook |
| tc | 630.20 ± 0.80 | K | NIST Webbook |
| tc | 629.60 ± 0.50 | K | NIST Webbook |
| tc | 637.30 | K | NIST Webbook |
| tf | 225.74 | K | Joback Method |
| vc | 0.519 | m3/kmol | NIST Webbook |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 345.08 | J/mol×K | 609.94 | Joback Method |
| cpg | 324.43 | J/mol×K | 555.64 | Joback Method |
| cpg | 313.47 | J/mol×K | 528.49 | Joback Method |
| cpg | 302.08 | J/mol×K | 501.33 | Joback Method |
| cpg | 290.23 | J/mol×K | 474.18 | Joback Method |
| cpg | 334.96 | J/mol×K | 582.79 | Joback Method |
| cpg | 354.79 | J/mol×K | 637.10 | Joback Method |
| cpl | 330.10 | J/mol×K | 298.50 | NIST Webbook |
| dvisc | 0.1178389 | Pa×s | 225.74 | Joback Method |
| dvisc | 0.0001689 | Pa×s | 474.18 | Joback Method |
| dvisc | 0.0002984 | Pa×s | 432.77 | Joback Method |
| dvisc | 0.0005948 | Pa×s | 391.37 | Joback Method |
| dvisc | 0.0013956 | Pa×s | 349.96 | Joback Method |
| dvisc | 0.0041171 | Pa×s | 308.55 | Joback Method |
| dvisc | 0.0169844 | Pa×s | 267.15 | Joback Method |
| hvapt | 60.00 | kJ/mol | 399.00 | NIST Webbook |
| hvapt | 60.70 | kJ/mol | 393.00 | NIST Webbook |
| hvapt | 70.70 | kJ/mol | 303.00 | NIST Webbook |
| hvapt | 56.10 | kJ/mol | 410.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 2.02089e+02 |
| Coeff. B | -1.56587e+04 |
| Coeff. C | -2.70414e+01 |
| Coeff. D | 1.21802e-05 |
| Temperature range (K), min. | 241.55 |
| Temperature range (K), max. | 637.15 |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C123966&Units=SI |
| **KDB Vapor Pressure Data:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=842 |
| **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 |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **cpl:** | Liquid phase 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 |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |

| | |
|---|---|
| **rhoc:** | Critical density |
| **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 |