# 3-Octanone

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|---|---|
| **Other names:** | 3-Oxooctane |
| | 3-octanonere |
| | Amyl ethyl ketone |
| | EAK |
| | Ethyl amyl ketone |
| | Ethyl n-amyl ketone |
| | Ethyl n-pentyl ketone |
| | Ethyl pentyl ketone |
| | NSC 60161 |
| | Octan-3-one |
| | n-Octanone-3 |
| **Inchi:** | InChI=1S/C8H16O/c1-3-5-6-7-8(9)4-2/h3-7H2,1-2H3 |
| **InchiKey:** | RHLVCLIPMVJYKS-UHFFFAOYSA-N |
| **Formula:** | C8H16O |
| **SMILES:** | CCCCCC(=O)CC |
| **Mol. weight [g/mol]:** | 128.21 |
| **CAS:** | 106-68-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chl | -5052.01 | kJ/mol | NIST Webbook |
| gf | -112.44 | kJ/mol | Joback Method |
| hf | -338.60 ± 3.30 | kJ/mol | NIST Webbook |
| hfus | 18.07 | kJ/mol | Joback Method |
| hvap | 44.40 ± 0.20 | kJ/mol | NIST Webbook |
| log10ws | -2.45 | | Crippen Method |
| logp | 2.546 | | Crippen Method |
| mcvol | 125.150 | ml/mol | McGowan Method |
| pc | 2704.22 | kPa | Joback Method |
| rhoc | 257.71 ± 2.56 | kg/m3 | NIST Webbook |
| rinpol | 986.00 | | NIST Webbook |
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| tb | 436.31 | K | Joback Method |
| tc | 627.70 ± 0.20 | K | NIST Webbook |
| tf | 229.85 | K | Joback Method |
| vc | 0.489 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 313.17 | J/mol×K | 582.49 | Joback Method |
| cpg | 302.57 | J/mol×K | 553.25 | Joback Method |
| cpg | 291.52 | J/mol×K | 524.02 | Joback Method |
| cpg | 280.00 | J/mol×K | 494.78 | Joback Method |
| cpg | 267.99 | J/mol×K | 465.55 | Joback Method |
| cpg | 255.50 | J/mol×K | 436.31 | Joback Method |
| cpg | 323.31 | J/mol×K | 611.72 | Joback Method |
| dvisc | 0.0043730 | Pa×s | 229.85 | Joback Method |
| dvisc | 0.0002948 | Pa×s | 436.31 | Joback Method |
| dvisc | 0.0003813 | Pa×s | 401.90 | Joback Method |
| dvisc | 0.0005173 | Pa×s | 367.49 | Joback Method |
| dvisc | 0.0007477 | Pa×s | 333.08 | Joback Method |
| dvisc | 0.0011762 | Pa×s | 298.67 | Joback Method |
| dvisc | 0.0020821 | Pa×s | 264.26 | Joback Method |
| hvapt | 43.80 | kJ/mol | 320.50 | NIST Webbook |
| rhol | 817.77 | kg/m3 | 298.15 | Excess Molar Enthalpies of Binary Systems of 2-Octanone or 3-Octanone with Dodecane, Tetradecane, or Hexadecane at 298.15 K |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.52035e+01 |

| | |
|---|---|
| Coeff. B | -3.97315e+03 |
| Coeff. C | -6.36510e+01 |
| Temperature range (K), min. | 330.02 |
| Temperature range (K), max. | 465.30 |

# Sources

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|---|---|
| **Excess Molar Enthalpies of Binary Systems of 2-Octanone or 3-Octanone with Dodecane, Tetradecane, or Hexadecane at 298.15 K:** | https://www.doi.org/10.1021/je900311v |
| **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=C106683&Units=SI |
| **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 |

# Legend

| | |
|---|---|
| **chl:** | Standard liquid enthalpy of combustion |
| **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 |
| **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 |
| **rhol:** | Liquid 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 |