# 5-Dodecanone

**Other names:** Butyl heptyl ketone
dodecan-5-one
n-Butyl n-heptyl ketone
**Inchi:** InChI=1S/C12H24O/c1-3-5-7-8-9-11-12(13)10-6-4-2/h3-11H2,1-2H3
**InchiKey:** DOXYUCZSYSEALW-UHFFFAOYSA-N
**Formula:** C12H24O
**SMILES:** CCCCCCCC(=O)CCCC
**Mol. weight [g/mol]:** 184.32
**CAS:** 19780-10-0

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -78.76 | kJ/mol | Joback Method |
| hf | -403.59 | kJ/mol | Joback Method |
| hfus | 28.43 | kJ/mol | Joback Method |
| hvap | 49.05 | kJ/mol | Joback Method |
| log10ws | -4.13 | | Crippen Method |
| logp | 4.106 | | Crippen Method |
| mcvol | 181.510 | ml/mol | McGowan Method |
| pc | 1878.90 | kPa | Joback Method |
| rhoc | 243.30 ± 7.37 | kg/m3 | NIST Webbook |
| tb | 527.83 | K | Joback Method |
| tc | 695.20 ± 3.00 | K | NIST Webbook |
| tf | 282.85 ± 2.00 | K | NIST Webbook |
| vc | 0.714 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 436.30 | J/mol×K | 527.83 | Joback Method |
| cpg | 509.69 | J/mol×K | 669.65 | Joback Method |
| cpg | 496.25 | J/mol×K | 641.28 | Joback Method |
| cpg | 482.21 | J/mol×K | 612.92 | Joback Method |
| cpg | 467.55 | J/mol×K | 584.56 | Joback Method |

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|---|---|---|---|---|
| cpg | 452.25 | J/mol×K | 556.19 | Joback Method |
| cpg | 522.54 | J/mol×K | 698.01 | Joback Method |
| dvisc | 0.0002319 | Pa×s | 527.83 | Joback Method |
| dvisc | 0.0003061 | Pa×s | 485.68 | Joback Method |
| dvisc | 0.0004257 | Pa×s | 443.53 | Joback Method |
| dvisc | 0.0006347 | Pa×s | 401.38 | Joback Method |
| dvisc | 0.0010391 | Pa×s | 359.23 | Joback Method |
| dvisc | 0.0019395 | Pa×s | 317.08 | Joback Method |
| dvisc | 0.0043838 | Pa×s | 274.93 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.52621e+01 |
| Coeff. B | -4.59344e+03 |
| Coeff. C | -8.48900e+01 |
| Temperature range (K), min. | 391.64 |
| Temperature range (K), max. | 546.51 |

# Sources

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|---|---|
| **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=C19780100&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

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |

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|---|---|
| **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 |
| **rhoc:** | Critical density |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |