# 2-Methyl-4-decanone

**Inchi:** InChI=1S/C11H22O/c1-4-5-6-7-8-11(12)9-10(2)3/h10H,4-9H2,1-3H3
**InchiKey:** QNIWMSRDAQBYHO-UHFFFAOYSA-N
**Formula:** C11H22O
**SMILES:** CCCCCCC(=O)CC(C)C
**Mol. weight [g/mol]:** 170.29
**CAS:** 6628-25-7

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -89.62 | kJ/mol | Joback Method |
| hf | -388.23 | kJ/mol | Joback Method |
| hfus | 22.32 | kJ/mol | Joback Method |
| hvap | 46.44 | kJ/mol | Joback Method |
| log10ws | -3.47 | | Crippen Method |
| logp | 3.572 | | Crippen Method |
| mcvol | 167.420 | ml/mol | McGowan Method |
| pc | 2060.49 | kPa | Joback Method |
| tb | 504.51 | K | Joback Method |
| tc | 679.38 | K | Joback Method |
| tf | 248.66 | K | Joback Method |
| vc | 0.651 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 388.41 | J/mol×K | 504.51 | Joback Method |
| cpg | 404.02 | J/mol×K | 533.65 | Joback Method |
| cpg | 418.97 | J/mol×K | 562.80 | Joback Method |
| cpg | 433.29 | J/mol×K | 591.94 | Joback Method |
| cpg | 446.99 | J/mol×K | 621.09 | Joback Method |
| cpg | 460.10 | J/mol×K | 650.23 | Joback Method |
| cpg | 472.61 | J/mol×K | 679.38 | Joback Method |
| dvisc | 0.0065882 | Pa×s | 248.66 | Joback Method |
| dvisc | 0.0025234 | Pa×s | 291.30 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0012349 | Pa×s | 333.94 | Joback Method |
| dvisc | 0.0007105 | Pa×s | 376.59 | Joback Method |
| dvisc | 0.0004574 | Pa×s | 419.23 | Joback Method |
| dvisc | 0.0003195 | Pa×s | 461.87 | Joback Method |
| dvisc | 0.0002371 | Pa×s | 504.51 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.45783e+01 |
| Coeff. B | -4.18822e+03 |
| Coeff. C | -7.76060e+01 |
| Temperature range (K), min. | 370.68 |
| Temperature range (K), max. | 529.57 |

# 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

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C6628257&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |