# 2-Octanone, 7-methyl-

**Other names:** 7-methyl-2-octanone
7-methyloctan-2-one
**Inchi:** InChI=1S/C9H18O/c1-8(2)6-4-5-7-9(3)10/h8H,4-7H2,1-3H3
**InchiKey:** OPSQVVYXYQMUEV-UHFFFAOYSA-N
**Formula:** C9H18O
**SMILES:** CC(=O)CCCCC(C)C
**Mol. weight [g/mol]:** 142.24
**CAS:** 1482-13-9

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -106.46 | kJ/mol | Joback Method |
| hf | -346.95 | kJ/mol | Joback Method |
| hfus | 17.14 | kJ/mol | Joback Method |
| hvap | 41.99 | kJ/mol | Joback Method |
| log10ws | -2.63 | | Crippen Method |
| logp | 2.792 | | Crippen Method |
| mcvol | 139.240 | ml/mol | McGowan Method |
| pc | 2472.73 | kPa | Joback Method |
| rinpol | 1057.00 | | NIST Webbook |
| rinpol | 1057.00 | | NIST Webbook |
| ripol | 1337.00 | | NIST Webbook |
| tb | 458.75 | K | Joback Method |
| tc | 636.64 | K | Joback Method |
| tf | 226.12 | K | Joback Method |
| vc | 0.539 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 297.82 | J/mol×K | 458.75 | Joback Method |
| cpg | 311.71 | J/mol×K | 488.40 | Joback Method |
| cpg | 325.02 | J/mol×K | 518.05 | Joback Method |
| cpg | 337.78 | J/mol×K | 547.69 | Joback Method |

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|---|---|---|---|---|
| cpg | 350.00 | J/mol×K | 577.34 | Joback Method |
| cpg | 361.70 | J/mol×K | 606.99 | Joback Method |
| cpg | 372.87 | J/mol×K | 636.64 | Joback Method |
| dvisc | 0.0068479 | Pa×s | 226.12 | Joback Method |
| dvisc | 0.0026929 | Pa×s | 264.89 | Joback Method |
| dvisc | 0.0013439 | Pa×s | 303.66 | Joback Method |
| dvisc | 0.0007850 | Pa×s | 342.44 | Joback Method |
| dvisc | 0.0005116 | Pa×s | 381.21 | Joback Method |
| dvisc | 0.0003608 | Pa×s | 419.98 | Joback Method |
| dvisc | 0.0002699 | Pa×s | 458.75 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.46970e+01 |
| Coeff. B | -3.93944e+03 |
| Coeff. C | -6.71260e+01 |
| Temperature range (K), min. | 340.52 |
| Temperature range (K), max. | 486.86 |

# 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=C1482139&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 |