# 11-Hentriacontanone

**Inchi:** InChI=1S/C31H62O/c1-3-5-7-9-11-13-14-15-16-17-18-19-20-21-22-24-26-28-30-31(32)2
**InchiKey:** MQCASZXGPSJCPY-UHFFFAOYSA-N
**Formula:** C31H62O
**SMILES:** CCCCCCCCCCCCCCCCCCCCC(=O)CCCCCCCCCC
**Mol. weight [g/mol]:** 450.82
**CAS:** 1201402-84-7

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 81.22 | kJ/mol | Joback Method |
| hf | -795.75 | kJ/mol | Joback Method |
| hfus | 77.65 | kJ/mol | Joback Method |
| hvap | 91.35 | kJ/mol | Joback Method |
| log10ws | -12.08 | | Crippen Method |
| logp | 11.518 | | Crippen Method |
| mcvol | 449.220 | ml/mol | McGowan Method |
| pc | 585.99 | kPa | Joback Method |
| rinpol | 3304.90 | | NIST Webbook |
| rinpol | 3304.90 | | NIST Webbook |
| tb | 962.55 | K | Joback Method |
| tc | 1197.11 | K | Joback Method |
| tf | 489.06 | K | Joback Method |
| vc | 1.778 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1581.38 | J/mol×K | 962.55 | Joback Method |
| cpg | 1701.41 | J/mol×K | 1158.02 | Joback Method |
| cpg | 1680.55 | J/mol×K | 1118.92 | Joback Method |
| cpg | 1658.24 | J/mol×K | 1079.83 | Joback Method |
| cpg | 1634.36 | J/mol×K | 1040.74 | Joback Method |
| cpg | 1608.78 | J/mol×K | 1001.64 | Joback Method |
| cpg | 1720.95 | J/mol×K | 1197.11 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000196 | Pa×s | 962.55 | Joback Method |
| dvisc | 0.0000271 | Pa×s | 883.63 | Joback Method |
| dvisc | 0.0000398 | Pa×s | 804.72 | Joback Method |
| dvisc | 0.0000636 | Pa×s | 725.80 | Joback Method |
| dvisc | 0.0001141 | Pa×s | 646.89 | Joback Method |
| dvisc | 0.0002408 | Pa×s | 567.98 | Joback Method |
| dvisc | 0.0006463 | Pa×s | 489.06 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1201402847&Units=SI |
| **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 |

# Legend

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|---|---|
| **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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |