# 9-Hexadecenoic acid

**Inchi:** InChI=1S/C16H30O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16(17)18/h7-8H,2-6,9-15H2
**InchiKey:** SECPZKHBENQXJG-BQYQJAHWSA-N
**Formula:** C16H30O2
**SMILES:** CCCCCCC=CCCCCCCCC(=O)O
**Mol. weight [g/mol]:** 254.41
**CAS:** 2091-29-4

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -101.68 | kJ/mol | Joback Method |
| hf | -521.16 | kJ/mol | Joback Method |
| hfus | 43.09 | kJ/mol | Joback Method |
| hvap | 74.59 | kJ/mol | Joback Method |
| log10ws | -5.47 | | Crippen Method |
| logp | 5.328 | | Crippen Method |
| mcvol | 239.440 | ml/mol | McGowan Method |
| pc | 1541.49 | kPa | Joback Method |
| rinpol | 1916.29 | | NIST Webbook |
| rinpol | 1942.00 | | NIST Webbook |
| rinpol | 1948.00 | | NIST Webbook |
| rinpol | 1938.00 | | NIST Webbook |
| rinpol | 1911.00 | | NIST Webbook |
| rinpol | 1942.00 | | NIST Webbook |
| rinpol | 1949.00 | | NIST Webbook |
| rinpol | 1949.00 | | NIST Webbook |
| rinpol | 1957.00 | | NIST Webbook |
| rinpol | 1898.00 | | NIST Webbook |
| rinpol | 1898.00 | | NIST Webbook |
| rinpol | 1942.00 | | NIST Webbook |
| ripol | 2950.00 | | NIST Webbook |
| ripol | 2957.00 | | NIST Webbook |
| ripol | 2950.00 | | NIST Webbook |
| tb | 715.69 | K | Joback Method |
| tc | 887.89 | K | Joback Method |
| tf | 375.75 | K | Joback Method |
| vc | 0.936 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 696.79 | J/mol×K | 715.69 | Joback Method |
| cpg | 712.23 | J/mol×K | 744.39 | Joback Method |
| cpg | 726.95 | J/mol×K | 773.09 | Joback Method |
| cpg | 740.99 | J/mol×K | 801.79 | Joback Method |
| cpg | 754.38 | J/mol×K | 830.49 | Joback Method |
| cpg | 767.14 | J/mol×K | 859.19 | Joback Method |
| cpg | 779.32 | J/mol×K | 887.89 | Joback Method |
| dvisc | 0.0034930 | Pa×s | 375.75 | Joback Method |
| dvisc | 0.0009417 | Pa×s | 432.41 | Joback Method |
| dvisc | 0.0003440 | Pa×s | 489.06 | Joback Method |
| dvisc | 0.0001549 | Pa×s | 545.72 | Joback Method |
| dvisc | 0.0000810 | Pa×s | 602.38 | Joback Method |
| dvisc | 0.0000474 | Pa×s | 659.03 | Joback Method |
| dvisc | 0.0000302 | Pa×s | 715.69 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.46024e+01 |
| Coeff. B | -5.30092e+03 |
| Coeff. C | -1.16610e+02 |
| Temperature range (K), min. | 486.92 |
| Temperature range (K), max. | 687.16 |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C2091294&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 |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |