# 1-Heptacosene

**Inchi:** InChI=1S/C27H54/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-26-24-22-20-18-16-14-12-10-
**InchiKey:** YYLACZAXCCJCJO-UHFFFAOYSA-N
**Formula:** C27H54
**SMILES:** C=CCCCCCCCCCCCCCCCCCCCCCCCCC
**Mol. weight [g/mol]:** 378.72
**CAS:** 15306-27-1

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 264.30 | kJ/mol | Joback Method |
| hf | -475.18 | kJ/mol | Joback Method |
| hfus | 64.41 | kJ/mol | Joback Method |
| hvap | 75.03 | kJ/mol | Joback Method |
| log10ws | -10.98 | | Crippen Method |
| logp | 10.555 | | Crippen Method |
| mcvol | 386.990 | ml/mol | McGowan Method |
| pc | 704.33 | kPa | Joback Method |
| rinpol | 2694.00 | | NIST Webbook |
| rinpol | 2684.20 | | NIST Webbook |
| rinpol | 2684.20 | | NIST Webbook |
| rinpol | 2693.00 | | NIST Webbook |
| rinpol | 2688.00 | | NIST Webbook |
| tb | 813.84 | K | Joback Method |
| tc | 996.48 | K | Joback Method |
| tf | 392.29 | K | Joback Method |
| vc | 1.528 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1253.98 | J/mol×K | 813.84 | Joback Method |
| cpg | 1278.03 | J/mol×K | 844.28 | Joback Method |
| cpg | 1300.90 | J/mol×K | 874.72 | Joback Method |
| cpg | 1322.65 | J/mol×K | 905.16 | Joback Method |

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|---|---|---|---|---|
| cpg | 1343.32 | J/mol×K | 935.60 | Joback Method |
| cpg | 1362.98 | J/mol×K | 966.04 | Joback Method |
| cpg | 1381.67 | J/mol×K | 996.48 | Joback Method |
| dvisc | 0.0016041 | Pa×s | 392.29 | Joback Method |
| dvisc | 0.0005451 | Pa×s | 462.55 | Joback Method |
| dvisc | 0.0002462 | Pa×s | 532.81 | Joback Method |
| dvisc | 0.0001338 | Pa×s | 603.07 | Joback Method |
| dvisc | 0.0000826 | Pa×s | 673.32 | Joback Method |
| dvisc | 0.0000559 | Pa×s | 743.58 | Joback Method |
| dvisc | 0.0000404 | Pa×s | 813.84 | Joback Method |
| hvapt | 108.70 | kJ/mol | 567.50 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.25286e+01 |
| Coeff. B | -3.63313e+03 |
| Coeff. C | -2.30607e+02 |
| Temperature range (K), min. | 527.41 |
| Temperature range (K), max. | 734.01 |

# 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=C15306271&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 |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |