# 11-Phenylheneicosane

**Other names:** Benzene, heneicosyl-
**Inchi:** InChI=1S/C27H48/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-21-24-27-25-22-2
**InchiKey:** OWXCBZFAHWMZCQ-UHFFFAOYSA-N
**Formula:** C27H48
**SMILES:** CCCCCCCCCCCCCCCCCCCCCc1ccccc1
**Mol. weight [g/mol]:** 372.68
**CAS:** 6703-80-6

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 1.0591 | | Cheméo Relay (1.0) |
| chl | -16980.80 ± 6.70 | kJ/mol | NIST Webbook |
| chl | -16977.80 ± 6.70 | kJ/mol | NIST Webbook |
| gf | 288.87 | kJ/mol | Joback Method |
| hf | -355.76 | kJ/mol | Cheméo Relay (1.0) |
| hfl | -506.80 ± 6.70 | kJ/mol | NIST Webbook |
| hfl | -508.10 ± 6.70 | kJ/mol | NIST Webbook |
| hfus | 59.73 | kJ/mol | Joback Method |
| hvap | 132.04 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.31 | eV | Cheméo Relay (1.0) |
| log10ws | -9.68 | | Cheméo Relay (1.0) |
| logp | 9.661 | | Crippen Method |
| mcvol | 367.530 | ml/mol | McGowan Method |
| pc | 826.21 | kPa | Joback Method |
| tb | 651.84 | K | Cheméo Relay (1.0) |
| tc | 836.19 | K | Cheméo Relay (1.0) |
| tf | 306.14 | K | Cheméo Relay (1.0) |
| vc | 1.451 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1295.31 | J/mol×K | 1002.85 | Joback Method |
| cpg | 1312.07 | J/mol×K | 1034.66 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 1218.17 | J/mol×K | 875.64 | Joback Method |
| cpg | 1239.09 | J/mol×K | 907.45 | Joback Method |
| cpg | 1258.88 | J/mol×K | 939.25 | Joback Method |
| cpg | 1277.60 | J/mol×K | 971.05 | Joback Method |
| cpg | 1196.03 | J/mol×K | 843.84 | Joback Method |
| dvisc | 0.0002163 | Pa×s | 561.59 | Joback Method |
| dvisc | 0.0004526 | Pa×s | 491.03 | Joback Method |
| dvisc | 0.0012137 | Pa×s | 420.47 | Joback Method |
| dvisc | 0.0001219 | Pa×s | 632.15 | Joback Method |
| dvisc | 0.0000770 | Pa×s | 702.72 | Joback Method |
| dvisc | 0.0000530 | Pa×s | 773.28 | Joback Method |
| dvisc | 0.0000388 | Pa×s | 843.84 | Joback Method |
| hvapt | 108.40 | kJ/mol | 575.50 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.40815e+01 |
| Coeff. B | -5.44421e+03 |
| Coeff. C | -1.34916e+02 |
| Temperature range (K), min. | 529.60 |
| Temperature range (K), max. | 755.69 |

# Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**Cheméo Relay (1.0):**

**Cheméo Relay (1.0, beta):**

**The Yaws Handbook of Vapor Pressure:** https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C40775095&Units=SI

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

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

# Legend

| | |
|---|---|
| **af:** | Acentric Factor |
| **chl:** | Standard liquid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfl:** | Liquid phase 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 |
| **ie:** | Ionization energy |
| **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 |