# HEXADECANOPHENONE

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|---|---|
| **Other names:** | Pentadecyl phenyl ketone |
| | n-Hexadecanophenone |
| | 1-Hexadecanone, 1-phenyl- |
| **Inchi:** | InChI=1S/C22H36O/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-20-22(23)21-18-15-14-16-19-21/ |
| **InchiKey:** | IIOLAWJMOGLOIB-UHFFFAOYSA-N |
| **Formula:** | C22H36O |
| **SMILES:** | CCCCCCCCCCCCCCCC(=O)c1ccccc1 |
| **Mol. weight [g/mol]:** | 316.53 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.9438 | | Cheméo Relay (1.0) |
| gf | 117.85 | kJ/mol | Joback Method |
| hf | -388.52 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 48.38 | kJ/mol | Joback Method |
| hvap | 112.56 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.41 | eV | Cheméo Relay (1.0) |
| log10ws | -7.44 | | Cheméo Relay (1.0) |
| logp | 7.351 | | Crippen Method |
| mcvol | 298.650 | ml/mol | McGowan Method |
| pc | 1160.08 | kPa | Joback Method |
| tb | 630.64 | K | Cheméo Relay (1.0) |
| tc | 839.00 | K | Cheméo Relay (1.0) |
| tf | 324.00 ± 3.00 | K | NIST Webbook |
| tf | 332.20 ± 0.60 | K | NIST Webbook |
| vc | 1.144 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 913.68 | J/mol×K | 783.31 | Joback Method |
| cpg | 932.83 | J/mol×K | 815.02 | Joback Method |
| cpg | 950.90 | J/mol×K | 846.72 | Joback Method |
| cpg | 967.96 | J/mol×K | 878.43 | Joback Method |

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|---|---|---|---|---|
| cpg | 984.04 | J/mol×K | 910.13 | Joback Method |
| cpg | 999.21 | J/mol×K | 941.84 | Joback Method |
| cpg | 1013.52 | J/mol×K | 973.54 | Joback Method |
| dvisc | 0.0015501 | Pa×s | 414.05 | Joback Method |
| dvisc | 0.0006747 | Pa×s | 475.59 | Joback Method |
| dvisc | 0.0003553 | Pa×s | 537.14 | Joback Method |
| dvisc | 0.0002135 | Pa×s | 598.68 | Joback Method |
| dvisc | 0.0001411 | Pa×s | 660.22 | Joback Method |
| dvisc | 0.0001000 | Pa×s | 721.77 | Joback Method |
| dvisc | 0.0000749 | Pa×s | 783.31 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 521.20 | K | 1.60 | NIST Webbook |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C6697127&Units=SI
**Joback Method:** https://en.wikipedia.org/wiki/Joback_method
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**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):**

# Legend

**af:** Acentric Factor
**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

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|---|---|
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |