# Hexadecane, 2,6,10,14-tetramethyl-

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|---|---|
| **Other names:** | Phytan |
| | Phytane |
| | 2,6,10,14-Tetramethylhexadecane |
| | 2,6,10,14-Tetramethylhexadecane (phytane) |
| **Inchi:** | InChI=1S/C20H42/c1-7-18(4)12-9-14-20(6)16-10-15-19(5)13-8-11-17(2)3/h17-20H,7-16H |
| **InchiKey:** | GGYKPYDKXLHNTI-UHFFFAOYSA-N |
| **Formula:** | C20H42 |
| **SMILES:** | CCC(C)CCCC(C)CCCC(C)CCCC(C)C |
| **Mol. weight [g/mol]:** | 282.55 |
| **CAS:** | 638-36-8 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 107.76 | kJ/mol | Joback Method |
| hf | -477.25 | kJ/mol | Joback Method |
| hfus | 33.46 | kJ/mol | Joback Method |
| hvap | 58.56 | kJ/mol | Joback Method |
| log10ws | -7.23 | | Crippen Method |
| logp | 7.472 | | Crippen Method |
| mcvol | 292.660 | ml/mol | McGowan Method |
| pc | 1036.57 | kPa | Joback Method |
| rinpol | 1787.00 | | NIST Webbook |
| rinpol | 1811.00 | | NIST Webbook |
| rinpol | 1795.00 | | NIST Webbook |
| rinpol | 1789.00 | | NIST Webbook |
| rinpol | 1814.00 | | NIST Webbook |
| rinpol | 1800.00 | | NIST Webbook |
| rinpol | 1814.00 | | NIST Webbook |
| rinpol | 1791.00 | | NIST Webbook |
| rinpol | 1786.60 | | NIST Webbook |
| rinpol | 1811.00 | | NIST Webbook |
| rinpol | 1814.00 | | NIST Webbook |
| rinpol | 1790.00 | | NIST Webbook |
| rinpol | 1814.00 | | NIST Webbook |
| rinpol | 1791.00 | | NIST Webbook |
| rinpol | 1811.00 | | NIST Webbook |
| rinpol | 1787.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 1789.00 | | NIST Webbook |
| rinpol | 1790.00 | | NIST Webbook |
| rinpol | 1791.00 | | NIST Webbook |
| rinpol | 1792.00 | | NIST Webbook |
| rinpol | 1793.00 | | NIST Webbook |
| rinpol | 298.42 | | NIST Webbook |
| rinpol | 1809.50 | | NIST Webbook |
| rinpol | 1815.00 | | NIST Webbook |
| rinpol | 1816.00 | | NIST Webbook |
| rinpol | 1812.00 | | NIST Webbook |
| rinpol | 1811.00 | | NIST Webbook |
| rinpol | 1795.00 | | NIST Webbook |
| rinpol | 1804.00 | | NIST Webbook |
| rinpol | 1809.00 | | NIST Webbook |
| rinpol | 1816.00 | | NIST Webbook |
| rinpol | 1813.00 | | NIST Webbook |
| rinpol | 1789.00 | | NIST Webbook |
| rinpol | 1808.00 | | NIST Webbook |
| rinpol | 1811.00 | | NIST Webbook |
| rinpol | 1806.00 | | NIST Webbook |
| rinpol | 1815.00 | | NIST Webbook |
| rinpol | 1812.00 | | NIST Webbook |
| rinpol | 1810.00 | | NIST Webbook |
| rinpol | 1792.00 | | NIST Webbook |
| rinpol | 1811.00 | | NIST Webbook |
| rinpol | 1812.00 | | NIST Webbook |
| rinpol | 1791.00 | | NIST Webbook |
| rinpol | 1810.70 | | NIST Webbook |
| rinpol | 303.08 | | NIST Webbook |
| rinpol | 1793.00 | | NIST Webbook |
| tb | 655.24 | K | Joback Method |
| tc | 822.89 | K | Joback Method |
| tf | 255.16 | K | Joback Method |
| vc | 1.131 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 841.81 | J/mol×K | 655.24 | Joback Method |
| cpg | 863.83 | J/mol×K | 683.18 | Joback Method |
| cpg | 884.89 | J/mol×K | 711.12 | Joback Method |

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|---|---|---|---|---|
| cpg | 905.01 | J/mol×K | 739.06 | Joback Method |
| cpg | 924.24 | J/mol×K | 767.00 | Joback Method |
| cpg | 942.58 | J/mol×K | 794.94 | Joback Method |
| cpg | 960.09 | J/mol×K | 822.89 | Joback Method |
| dvisc | 0.0197594 | Pa×s | 255.16 | Joback Method |
| dvisc | 0.0029435 | Pa×s | 321.84 | Joback Method |
| dvisc | 0.0008429 | Pa×s | 388.52 | Joback Method |
| dvisc | 0.0003482 | Pa×s | 455.20 | Joback Method |
| dvisc | 0.0001803 | Pa×s | 521.88 | Joback Method |
| dvisc | 0.0001084 | Pa×s | 588.56 | Joback Method |
| dvisc | 0.0000722 | Pa×s | 655.24 | Joback Method |

# 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=C638368&Units=SI

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