# 1,3,3,7-tetramethylcycloheptene

**Inchi:** InChI=1S/C11H20/c1-9-6-5-7-11(3,4)8-10(9)2/h8-9H,5-7H2,1-4H3
**InchiKey:** UCPZTFJETUKZLI-UHFFFAOYSA-N
**Formula:** C11H20
**SMILES:** CC1=CC(C)(C)CCCC1C
**Mol. weight [g/mol]:** 152.28

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 61.22 | kJ/mol | Joback Method |
| hf | -181.00 | kJ/mol | Joback Method |
| hfus | 9.59 | kJ/mol | Joback Method |
| hvap | 40.18 | kJ/mol | Joback Method |
| log10ws | -3.69 | | Crippen Method |
| logp | 3.779 | | Crippen Method |
| mcvol | 150.690 | ml/mol | McGowan Method |
| pc | 2472.73 | kPa | Joback Method |
| rinpol | 1042.50 | | NIST Webbook |
| rinpol | 1042.50 | | NIST Webbook |
| tb | 474.61 | K | Joback Method |
| tc | 688.62 | K | Joback Method |
| tf | 250.53 | K | Joback Method |
| vc | 0.559 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 333.04 | J/mol×K | 474.61 | Joback Method |
| cpg | 353.50 | J/mol×K | 510.28 | Joback Method |
| cpg | 372.75 | J/mol×K | 545.95 | Joback Method |
| cpg | 390.90 | J/mol×K | 581.62 | Joback Method |
| cpg | 408.02 | J/mol×K | 617.29 | Joback Method |
| cpg | 424.23 | J/mol×K | 652.96 | Joback Method |
| cpg | 439.62 | J/mol×K | 688.62 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R492049&Units=SI |
| **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

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |