# 1,4,4-trimethylcycloheptene

**Inchi:** InChI=1S/C10H18/c1-9-5-4-7-10(2,3)8-6-9/h6H,4-5,7-8H2,1-3H3
**InchiKey:** CPKYAUHXXUMQDM-UHFFFAOYSA-N
**Formula:** C10H18
**SMILES:** CC1=CCC(C)(C)CCC1
**Mol. weight [g/mol]:** 138.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 60.51 | kJ/mol | Joback Method |
| hf | -140.02 | kJ/mol | Joback Method |
| hfus | 5.93 | kJ/mol | Joback Method |
| hvap | 38.26 | kJ/mol | Joback Method |
| log10ws | -3.52 | | Crippen Method |
| logp | 3.533 | | Crippen Method |
| mcvol | 136.600 | ml/mol | McGowan Method |
| pc | 2823.32 | kPa | Joback Method |
| rinpol | 974.00 | | NIST Webbook |
| rinpol | 974.00 | | NIST Webbook |
| tb | 456.40 | K | Joback Method |
| tc | 673.85 | K | Joback Method |
| tf | 243.50 | K | Joback Method |
| vc | 0.504 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 287.14 | J/mol×K | 456.40 | Joback Method |
| cpg | 306.46 | J/mol×K | 492.64 | Joback Method |
| cpg | 324.55 | J/mol×K | 528.88 | Joback Method |
| cpg | 341.51 | J/mol×K | 565.12 | Joback Method |
| cpg | 357.45 | J/mol×K | 601.37 | Joback Method |
| cpg | 372.47 | J/mol×K | 637.61 | Joback Method |
| cpg | 386.67 | J/mol×K | 673.85 | 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=R492069&Units=SI |

# Legend

| | |
|---|---|
| **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 |