# 4-t-Butylcyclohexanone diethyl ketal

**Other names:** 4-tert-Butylcyclohexanone diethyl acetal
**Inchi:** InChI=1S/C14H28O2/c1-6-15-14(16-7-2)10-8-12(9-11-14)13(3,4)5/h12H,6-11H2,1-5H3
**InchiKey:** QTSXNUWFLGKEKB-UHFFFAOYSA-N
**Formula:** C14H28O2
**SMILES:** CCOC1(OCC)CCC(C(C)(C)C)CC1
**Mol. weight [g/mol]:** 228.37
**CAS:** 1900-58-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -128.91 | kJ/mol | Joback Method |
| hf | -556.26 | kJ/mol | Joback Method |
| hfus | 13.59 | kJ/mol | Joback Method |
| hvap | 49.25 | kJ/mol | Joback Method |
| log10ws | -3.88 | | Crippen Method |
| logp | 3.992 | | Crippen Method |
| mcvol | 209.000 | ml/mol | McGowan Method |
| pc | 1795.46 | kPa | Joback Method |
| tb | 576.45 | K | Joback Method |
| tc | 779.20 | K | Joback Method |
| tf | 321.46 | K | Joback Method |
| vc | 0.774 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 561.08 | J/mol×K | 576.45 | Joback Method |
| cpg | 583.45 | J/mol×K | 610.24 | Joback Method |
| cpg | 604.63 | J/mol×K | 644.03 | Joback Method |
| cpg | 624.72 | J/mol×K | 677.82 | Joback Method |
| cpg | 643.81 | J/mol×K | 711.61 | Joback Method |
| cpg | 661.99 | J/mol×K | 745.41 | Joback Method |
| cpg | 679.35 | J/mol×K | 779.20 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 402.50 ± 0.50 | K | 2.70 | NIST Webbook |

# Sources

| | |
|---|---|
| **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=C1900589&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |