# 1-carbomethoxy-1-methyl-3-tert-butylcyclohex-3-e

**Inchi:** InChI=1S/C13H22O2/c1-12(2,3)10-7-6-8-13(4,9-10)11(14)15-5/h7H,6,8-9H2,1-5H3
**InchiKey:** LDNSZCYDGAYSFG-UHFFFAOYSA-N
**Formula:** C13H22O2
**SMILES:** COC(=O)C1(C)CCC=C(C(C)(C)C)C1
**Mol. weight [g/mol]:** 210.31

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -133.21 | kJ/mol | Joback Method |
| hf | -449.33 | kJ/mol | Joback Method |
| hfus | 11.17 | kJ/mol | Joback Method |
| hvap | 52.62 | kJ/mol | Joback Method |
| log10ws | -3.39 | | Crippen Method |
| logp | 3.322 | | Crippen Method |
| mcvol | 186.310 | ml/mol | McGowan Method |
| pc | 2204.15 | kPa | Joback Method |
| ripol | 1676.90 | | NIST Webbook |
| tb | 593.83 | K | Joback Method |
| tc | 812.92 | K | Joback Method |
| tf | 355.41 | K | Joback Method |
| vc | 0.694 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 487.17 | J/mol×K | 593.83 | Joback Method |
| cpg | 506.28 | J/mol×K | 630.35 | Joback Method |
| cpg | 524.24 | J/mol×K | 666.86 | Joback Method |
| cpg | 541.18 | J/mol×K | 703.38 | Joback Method |
| cpg | 557.23 | J/mol×K | 739.89 | Joback Method |
| cpg | 572.52 | J/mol×K | 776.41 | Joback Method |
| cpg | 587.18 | J/mol×K | 812.92 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R388262&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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |