# trans-carbomethoxy-1,3-dimethylcyclohexane

**Inchi:** InChI=1S/C10H18O2/c1-8-5-4-6-10(2,7-8)9(11)12-3/h8H,4-7H2,1-3H3/t8-,10-/m1/s1
**InchiKey:** NOUTXABQGMIWME-PSASIEDQSA-N
**Formula:** C10H18O2
**SMILES:** COC(=O)C1(C)CCCC(C)C1
**Mol. weight [g/mol]:** 170.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -189.35 | kJ/mol | Joback Method |
| hf | -445.31 | kJ/mol | Joback Method |
| hfus | 11.05 | kJ/mol | Joback Method |
| hvap | 45.98 | kJ/mol | Joback Method |
| log10ws | -2.28 | | Crippen Method |
| logp | 2.376 | | Crippen Method |
| mcvol | 148.340 | ml/mol | McGowan Method |
| pc | 2726.86 | kPa | Joback Method |
| ripol | 1358.50 | | NIST Webbook |
| ripol | 1390.80 | | NIST Webbook |
| ripol | 1369.80 | | NIST Webbook |
| tb | 519.61 | K | Joback Method |
| tc | 733.33 | K | Joback Method |
| tf | 301.66 | K | Joback Method |
| vc | 0.549 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 355.82 | J/mol×K | 519.61 | Joback Method |
| cpg | 374.01 | J/mol×K | 555.23 | Joback Method |
| cpg | 391.16 | J/mol×K | 590.85 | Joback Method |
| cpg | 407.36 | J/mol×K | 626.47 | Joback Method |
| cpg | 422.69 | J/mol×K | 662.09 | Joback Method |
| cpg | 437.25 | J/mol×K | 697.71 | Joback Method |
| cpg | 451.12 | J/mol×K | 733.33 | Joback Method |

# Sources

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|---|---|
| **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=R388420&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |