# 2,3-dimethyl-4-isopropenyl-1-cyclopentanone

**Inchi:** InChI=1S/C10H16O/c1-6(2)9-5-10(11)8(4)7(9)3/h7-9H,1,5H2,2-4H3
**InchiKey:** CZUYJUUMDUMIDE-UHFFFAOYSA-N
**Formula:** C10H16O
**SMILES:** C=C(C)C1CC(=O)C(C)C1C
**Mol. weight [g/mol]:** 152.23

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 11.15 | kJ/mol | Joback Method |
| hf | -251.99 | kJ/mol | Joback Method |
| hfus | 14.65 | kJ/mol | Joback Method |
| hvap | 41.15 | kJ/mol | Joback Method |
| log10ws | -2.31 | | Crippen Method |
| logp | 2.424 | | Crippen Method |
| mcvol | 138.170 | ml/mol | McGowan Method |
| pc | 2545.61 | kPa | Joback Method |
| rinpol | 1113.00 | | NIST Webbook |
| tb | 498.52 | K | Joback Method |
| tc | 712.47 | K | Joback Method |
| tf | 257.38 | K | Joback Method |
| vc | 0.523 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 320.38 | J/mol×K | 498.52 | Joback Method |
| cpg | 338.69 | J/mol×K | 534.18 | Joback Method |
| cpg | 356.18 | J/mol×K | 569.84 | Joback Method |
| cpg | 372.84 | J/mol×K | 605.50 | Joback Method |
| cpg | 388.69 | J/mol×K | 641.15 | Joback Method |
| cpg | 403.71 | J/mol×K | 676.81 | Joback Method |
| cpg | 417.91 | J/mol×K | 712.47 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R187490&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

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

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