# Isoshyobunone

**Inchi:** InChI=1S/C15H24O/c1-7-15(6)9-8-12(10(2)3)14(16)13(15)11(4)5/h7,10,12H,1,8-9H2,2-6
**InchiKey:** YMIHAYABXZORPU-UHFFFAOYSA-N
**Formula:** C15H24O
**SMILES:** C=CC1(C)CCC(C(C)C)C(=O)C1=C(C)C
**Mol. weight [g/mol]:** 220.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 86.39 | kJ/mol | Joback Method |
| hf | -255.02 | kJ/mol | Joback Method |
| hfus | 14.93 | kJ/mol | Joback Method |
| hvap | 52.01 | kJ/mol | Joback Method |
| log10ws | -4.26 | | Crippen Method |
| logp | 4.150 | | Crippen Method |
| mcvol | 204.320 | ml/mol | McGowan Method |
| pc | 1854.71 | kPa | Joback Method |
| rinpol | 1518.00 | | NIST Webbook |
| rinpol | 1521.00 | | NIST Webbook |
| ripol | 1880.00 | | NIST Webbook |
| tb | 628.30 | K | Joback Method |
| tc | 851.27 | K | Joback Method |
| tf | 333.71 | K | Joback Method |
| vc | 0.771 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 552.73 | J/mol×K | 628.30 | Joback Method |
| cpg | 574.02 | J/mol×K | 665.46 | Joback Method |
| cpg | 594.20 | J/mol×K | 702.62 | Joback Method |
| cpg | 613.39 | J/mol×K | 739.79 | Joback Method |
| cpg | 631.70 | J/mol×K | 776.95 | Joback Method |
| cpg | 649.23 | J/mol×K | 814.11 | Joback Method |
| cpg | 666.10 | J/mol×K | 851.27 | Joback Method |

# 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=U360301&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 |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |