# Methyl 8,15-Isopimaradien-18-oate

**Inchi:** InChI=1S/C21H32O2/c1-6-19(2)13-10-16-15(14-19)8-9-17-20(16,3)11-7-12-21(17,4)18(2
**InchiKey:** GTFNGUBYWRFHMR-NRDMVMEKSA-N
**Formula:** C21H32O2
**SMILES:** C=CC1(C)CCC2=C(CCC3C(C)(C(=O)OC)CCCC23C)C1
**Mol. weight [g/mol]:** 316.48

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 88.13 | kJ/mol | Joback Method |
| hf | -348.32 | kJ/mol | Joback Method |
| hfus | 18.18 | kJ/mol | Joback Method |
| hvap | 69.28 | kJ/mol | Joback Method |
| log10ws | -5.90 | | Crippen Method |
| logp | 5.439 | | Crippen Method |
| mcvol | 273.010 | ml/mol | McGowan Method |
| pc | 1570.96 | kPa | Joback Method |
| rinpol | 2158.00 | | NIST Webbook |
| tb | 799.59 | K | Joback Method |
| tc | 1036.90 | K | Joback Method |
| tf | 526.31 | K | Joback Method |
| vc | 1.026 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 881.99 | J/mol×K | 799.59 | Joback Method |
| cpg | 908.01 | J/mol×K | 839.14 | Joback Method |
| cpg | 934.29 | J/mol×K | 878.69 | Joback Method |
| cpg | 961.27 | J/mol×K | 918.24 | Joback Method |
| cpg | 989.38 | J/mol×K | 957.79 | Joback Method |
| cpg | 1019.06 | J/mol×K | 997.34 | Joback Method |
| cpg | 1050.73 | J/mol×K | 1036.90 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R20491&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 |

# 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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