# (+)-Jasmonic acid, methyl ester (cis)

**Inchi:** InChI=1S/C13H20O3/c1-3-4-5-6-11-10(7-8-12(11)14)9-13(15)16-2/h4-5,10-11H,3,6-9H2,
**InchiKey:** GEWDNTWNSAZUDX-NRFYAWERSA-N
**Formula:** C13H20O3
**SMILES:** CCC=CCC1C(=O)CCC1CC(=O)OC
**Mol. weight [g/mol]:** 224.30

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -188.87 | kJ/mol | Joback Method |
| hf | -536.79 | kJ/mol | Joback Method |
| hfus | 26.93 | kJ/mol | Joback Method |
| hvap | 57.84 | kJ/mol | Joback Method |
| log10ws | -2.67 | | Crippen Method |
| logp | 2.501 | | Crippen Method |
| mcvol | 187.880 | ml/mol | McGowan Method |
| pc | 2092.66 | kPa | Joback Method |
| rinpol | 1632.00 | | NIST Webbook |
| rinpol | 1632.00 | | NIST Webbook |
| tb | 655.72 | K | Joback Method |
| tc | 866.01 | K | Joback Method |
| tf | 378.23 | K | Joback Method |
| vc | 0.715 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 522.90 | J/mol×K | 655.72 | Joback Method |
| cpg | 540.85 | J/mol×K | 690.77 | Joback Method |
| cpg | 557.79 | J/mol×K | 725.82 | Joback Method |
| cpg | 573.72 | J/mol×K | 760.87 | Joback Method |
| cpg | 588.65 | J/mol×K | 795.91 | Joback Method |
| cpg | 602.59 | J/mol×K | 830.96 | Joback Method |
| cpg | 615.53 | J/mol×K | 866.01 | Joback Method |

# Sources

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|---|---|
| **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=R169576&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |