# (-)-Jasmonic acid, Ile-conjugate # 2, methyl ester

**Inchi:** InChI=1S/C19H31NO4/c1-5-7-8-9-15-14(10-11-16(15)21)12-17(22)20-18(13(3)6-2)19(23

**InchiKey:** YAGOAONRDWKQSK-FPLPWBNLSA-N

**Formula:** C19H31NO4

**SMILES:** CCC=CCC1C(=O)CCC1CC(=O)NC(C(=O)OC)C(C)CC

**Mol. weight [g/mol]:** 337.45

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -182.76 | kJ/mol | Joback Method |
| hf | -730.30 | kJ/mol | Joback Method |
| hfus | 42.12 | kJ/mol | Joback Method |
| hvap | 83.60 | kJ/mol | Joback Method |
| log10ws | -4.02 | | Crippen Method |
| logp | 3.032 | | Crippen Method |
| mcvol | 283.970 | ml/mol | McGowan Method |
| pc | 1402.74 | kPa | Joback Method |
| rinpol | 2342.00 | | NIST Webbook |
| rinpol | 2342.00 | | NIST Webbook |
| tb | 896.16 | K | Joback Method |
| tc | 1109.88 | K | Joback Method |
| tf | 518.44 | K | Joback Method |
| vc | 1.079 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 948.27 | J/mol×K | 896.16 | Joback Method |
| cpg | 964.81 | J/mol×K | 931.78 | Joback Method |
| cpg | 979.93 | J/mol×K | 967.40 | Joback Method |
| cpg | 993.68 | J/mol×K | 1003.02 | Joback Method |
| cpg | 1006.06 | J/mol×K | 1038.64 | Joback Method |
| cpg | 1017.11 | J/mol×K | 1074.26 | Joback Method |
| cpg | 1026.85 | J/mol×K | 1109.88 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R539138&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

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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 |