# Homojasmonic acid, Ile conjugate, methyl ester

**Inchi:** InChI=1S/C20H33NO4/c1-5-7-8-9-16-15(10-12-17(16)22)11-13-18(23)21-19(14(3)6-2)20

**InchiKey:** KJUCNIXREXYKMO-QURVCBRASA-N

**Formula:** C20H33NO4

**SMILES:** CCC=CCC1C(=O)CCC1CCC(=O)NC(C(=O)OC)C(C)CC

**Mol. weight [g/mol]:** 351.48

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -174.34 | kJ/mol | Joback Method |
| hf | -750.94 | kJ/mol | Joback Method |
| hfus | 44.71 | kJ/mol | Joback Method |
| hvap | 85.83 | kJ/mol | Joback Method |
| log10ws | -4.44 | | Crippen Method |
| logp | 3.422 | | Crippen Method |
| mcvol | 298.060 | ml/mol | McGowan Method |
| pc | 1307.06 | kPa | Joback Method |
| rinpol | 2434.00 | | NIST Webbook |
| rinpol | 2434.00 | | NIST Webbook |
| tb | 919.04 | K | Joback Method |
| tc | 1133.58 | K | Joback Method |
| tf | 529.71 | K | Joback Method |
| vc | 1.135 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1008.74 | J/mol×K | 919.04 | Joback Method |
| cpg | 1025.30 | J/mol×K | 954.80 | Joback Method |
| cpg | 1040.41 | J/mol×K | 990.55 | Joback Method |
| cpg | 1054.08 | J/mol×K | 1026.31 | Joback Method |
| cpg | 1066.36 | J/mol×K | 1062.07 | Joback Method |
| cpg | 1077.27 | J/mol×K | 1097.83 | Joback Method |
| cpg | 1086.84 | J/mol×K | 1133.58 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R539198&Units=SI |

# 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 |