# Norchrysanthemic acid methyl ester

**Inchi:** InChI=1S/C10H16O2/c1-5-6-7-8(9(11)12-4)10(7,2)3/h5-8H,1-4H3
**InchiKey:** UKNHEHNRUOKYKB-UHFFFAOYSA-N
**Formula:** C10H16O2
**SMILES:** CC=CC1C(C(=O)OC)C1(C)C
**Mol. weight [g/mol]:** 168.23

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -80.54 | kJ/mol | Joback Method |
| hf | -329.95 | kJ/mol | Joback Method |
| hfus | 18.62 | kJ/mol | Joback Method |
| hvap | 45.11 | kJ/mol | Joback Method |
| log10ws | -1.89 | | Crippen Method |
| logp | 2.008 | | Crippen Method |
| mcvol | 144.040 | ml/mol | McGowan Method |
| pc | 2574.11 | kPa | Joback Method |
| rinpol | 1359.00 | | NIST Webbook |
| rinpol | 1359.00 | | NIST Webbook |
| tb | 506.29 | K | Joback Method |
| tc | 706.73 | K | Joback Method |
| tf | 302.90 | K | Joback Method |
| vc | 0.552 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 338.32 | J/mol×K | 506.29 | Joback Method |
| cpg | 353.68 | J/mol×K | 539.70 | Joback Method |
| cpg | 368.10 | J/mol×K | 573.10 | Joback Method |
| cpg | 381.70 | J/mol×K | 606.51 | Joback Method |
| cpg | 394.55 | J/mol×K | 639.92 | Joback Method |
| cpg | 406.77 | J/mol×K | 673.33 | Joback Method |
| cpg | 418.45 | J/mol×K | 706.73 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R593434&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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