# cis-Chrysanthenyl angelate

**Inchi:** InChI=1S/C15H22O2/c1-6-9(2)14(16)17-13-11-8-7-10(3)12(13)15(11,4)5/h6-7,11-13H,8H
**InchiKey:** XBIYGXBPWHLVBE-PXNMILOKSA-N
**Formula:** C15H22O2
**SMILES:** CC=C(C)C(=O)OC1C2CC=C(C)C1C2(C)C
**Mol. weight [g/mol]:** 234.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 21.99 | kJ/mol | Joback Method |
| hf | -329.99 | kJ/mol | Joback Method |
| hfus | 27.13 | kJ/mol | Joback Method |
| hvap | 57.36 | kJ/mol | Joback Method |
| log10ws | -3.85 | | Crippen Method |
| logp | 3.487 | | Crippen Method |
| mcvol | 199.330 | ml/mol | McGowan Method |
| pc | 1940.65 | kPa | Joback Method |
| rinpol | 1573.00 | | NIST Webbook |
| tb | 635.72 | K | Joback Method |
| tc | 848.11 | K | Joback Method |
| tf | 372.99 | K | Joback Method |
| vc | 0.768 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 553.17 | J/mol×K | 635.72 | Joback Method |
| cpg | 571.86 | J/mol×K | 671.12 | Joback Method |
| cpg | 589.55 | J/mol×K | 706.52 | Joback Method |
| cpg | 606.41 | J/mol×K | 741.92 | Joback Method |
| cpg | 622.57 | J/mol×K | 777.32 | Joback Method |
| cpg | 638.18 | J/mol×K | 812.71 | Joback Method |
| cpg | 653.38 | J/mol×K | 848.11 | Joback Method |

# Sources

| | |
|---|---|
| **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=R516031&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |