

# Chrysanthenyl acetate

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C12H18O2/c1-7-5-6-9-11(14-8(2)13)10(7)12(9,3)4/h5,9-11H,6H2,1-4H3/t9-,10-

UASZOTVHPVEMQR-OUAUKWLOSA-N

C12H18O2

CC(=O)OC1C2CC=C(C)C1C2(C)C

194.27

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -74.94  | kJ/mol  | Joback Method  |
| hf            | -375.50 | kJ/mol  | Joback Method  |
| hfus          | 20.47   | kJ/mol  | Joback Method  |
| hvap          | 50.64   | kJ/mol  | Joback Method  |
| log10ws       | -2.74   |         | Crippen Method |
| logp          | 2.540   |         | Crippen Method |
| mcvol         | 161.360 | ml/mol  | McGowan Method |
| pc            | 2405.28 | kPa     | Joback Method  |
| rinpol        | 1156.00 |         | NIST Webbook   |
| rinpol        | 1233.00 |         | NIST Webbook   |
| rinpol        | 1233.00 |         | NIST Webbook   |
| tb            | 563.04  | K       | Joback Method  |
| tc            | 773.40  | K       | Joback Method  |
| tf            | 358.22  | K       | Joback Method  |
| vc            | 0.620   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 419.92 | J/mol×K | 563.04          | Joback Method |
| cpg           | 437.32 | J/mol×K | 598.10          | Joback Method |
| cpg           | 453.71 | J/mol×K | 633.16          | Joback Method |
| cpg           | 469.20 | J/mol×K | 668.22          | Joback Method |
| cpg           | 483.90 | J/mol×K | 703.28          | Joback Method |
| cpg           | 497.94 | J/mol×K | 738.34          | Joback Method |
| cpg           | 511.43 | J/mol×K | 773.40          | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R633597&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R633597&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>                         |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |

# Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpola:</b> | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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