# Desmethoxyencecalin

**Other names:** 2,2-Dimethyl-6-acetyl-3-chromene
Demethoxyencecaline
**Inchi:** InChI=1S/C13H14O2/c1-9(14)10-4-5-12-11(8-10)6-7-13(2,3)15-12/h4-8H,1-3H3
**InchiKey:** ZAJTXVHECZCXLH-UHFFFAOYSA-N
**Formula:** C13H14O2
**SMILES:** CC(=O)c1ccc2c(c1)C=CC(C)(C)O2
**Mol. weight [g/mol]:** 202.25

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 9.81 | kJ/mol | Joback Method |
| hf | -202.98 | kJ/mol | Joback Method |
| hfus | 23.23 | kJ/mol | Joback Method |
| hvap | 58.61 | kJ/mol | Joback Method |
| log10ws | -3.92 | | Crippen Method |
| logp | 3.073 | | Crippen Method |
| mcvol | 162.550 | ml/mol | McGowan Method |
| pc | 2844.44 | kPa | Joback Method |
| rinpol | 1644.00 | | NIST Webbook |
| rinpol | 1646.00 | | NIST Webbook |
| rinpol | 1647.00 | | NIST Webbook |
| rinpol | 1657.00 | | NIST Webbook |
| rinpol | 1618.00 | | NIST Webbook |
| rinpol | 1657.00 | | NIST Webbook |
| rinpol | 1647.00 | | NIST Webbook |
| rinpol | 1646.00 | | NIST Webbook |
| ripol | 2401.00 | | NIST Webbook |
| ripol | 2401.00 | | NIST Webbook |
| ripol | 2418.00 | | NIST Webbook |
| ripol | 2449.00 | | NIST Webbook |
| tb | 624.71 | K | Joback Method |
| tc | 862.61 | K | Joback Method |
| tf | 403.31 | K | Joback Method |
| vc | 0.616 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 410.23 | J/mol×K | 624.71 | Joback Method |
| cpg | 425.15 | J/mol×K | 664.36 | Joback Method |
| cpg | 439.13 | J/mol×K | 704.01 | Joback Method |
| cpg | 452.36 | J/mol×K | 743.66 | Joback Method |
| cpg | 464.99 | J/mol×K | 783.31 | Joback Method |
| cpg | 477.22 | J/mol×K | 822.96 | Joback Method |
| cpg | 489.22 | J/mol×K | 862.61 | Joback Method |

# Sources

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|---|---|
| **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=R37656&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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