# 2H-Naphtho[1,2-b]pyran-5-carboxylate, 2,2-dimethyl-6-hydroxy-, methyl ester

**Other names:** Mollugin
**Inchi:** InChI=1S/C17H16O4/c1-17(2)9-8-12-13(16(19)20-3)14(18)10-6-4-5-7-11(10)15(12)21-17
**InchiKey:** VLGATXOTCNBWIT-UHFFFAOYSA-N
**Formula:** C17H16O4
**SMILES:** COC(=O)c1c2c(c3ccccc3c1O)OC(C)(C)C=C2
**Mol. weight [g/mol]:** 284.31
**CAS:** 55481-88-4

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -119.11 | kJ/mol | Joback Method |
| hf | -415.47 | kJ/mol | Joback Method |
| hfus | 37.19 | kJ/mol | Joback Method |
| hvap | 85.24 | kJ/mol | Joback Method |
| log10ws | -4.85 | | Crippen Method |
| logp | 3.516 | | Crippen Method |
| mcvol | 211.190 | ml/mol | McGowan Method |
| pc | 2778.85 | kPa | Joback Method |
| rinpol | 2237.00 | | NIST Webbook |
| rinpol | 2237.00 | | NIST Webbook |
| tb | 843.23 | K | Joback Method |
| tc | 1092.70 | K | Joback Method |
| tf | 627.56 | K | Joback Method |
| vc | 0.746 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 624.94 | J/mol×K | 843.23 | Joback Method |
| cpg | 640.31 | J/mol×K | 884.81 | Joback Method |
| cpg | 655.91 | J/mol×K | 926.39 | Joback Method |
| cpg | 672.02 | J/mol×K | 967.97 | Joback Method |
| cpg | 688.91 | J/mol×K | 1009.54 | Joback Method |
| cpg | 706.88 | J/mol×K | 1051.12 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 726.20 | J/mol×K | 1092.70 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C55481884&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |