# Phenol, 4-(3,4-dihydro-2,2,4-trimethyl-2H-1-benzopyran-4-

**Other names:** p-(2,2,4-Trimethyl-4-chromanyl)phenol
Dianin's compound
Phenol, p-(2,2,4-trimethyl-4-chromanyl)-
4-(4-Hydroxyphenyl)-2,2,4-trimethylchromane
4-(4'-Hydroxyphenyl)-2,2,4-trimethylchroman
4-p-Hydroxyphenyl-2,2,4-trimethylchroman
Chroman I
4-(4-Hydroxyphenyl)-2,2,4-trimethylchroman
2,2,4-Trimethyl-4-(4'-hydroxyphenyl)chroman
NSC 39757
p-(3,4-dihydro-2,2,4-trimethyl-2H-1-benzopyran-4-yl)phenol

**Inchi:** InChI=1S/C18H20O2/c1-17(2)12-18(3,13-8-10-14(19)11-9-13)15-6-4-5-7-16(15)20-17/h4

**InchiKey:** KXYDGGNWZUHESZ-UHFFFAOYSA-N

**Formula:** C18H20O2

**SMILES:** CC1(C)CC(C)(c2ccc(O)cc2)c2ccccc2O1

**Mol. weight [g/mol]:** 268.35

**CAS:** 472-41-3

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 105.09 | kJ/mol | Joback Method |
| hf | -185.79 | kJ/mol | Joback Method |
| hfus | 28.34 | kJ/mol | Joback Method |
| hvap | 75.87 | kJ/mol | Joback Method |
| log10ws | -4.59 | | Crippen Method |
| logp | 4.259 | | Crippen Method |
| mcvol | 217.840 | ml/mol | McGowan Method |
| pc | 2637.96 | kPa | Joback Method |
| tb | 783.97 | K | Joback Method |
| tc | 1050.23 | K | Joback Method |
| tf | 554.25 | K | Joback Method |
| vc | 0.758 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 648.34 | J/mol×K | 783.97 | Joback Method |
| cpg | 668.16 | J/mol×K | 828.35 | Joback Method |
| cpg | 688.31 | J/mol×K | 872.72 | Joback Method |
| cpg | 709.32 | J/mol×K | 917.10 | Joback Method |
| cpg | 731.70 | J/mol×K | 961.48 | Joback Method |
| cpg | 755.98 | J/mol×K | 1005.85 | Joback Method |
| cpg | 782.67 | J/mol×K | 1050.23 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C472413&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

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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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |