# Tocotrienol, 5-methyl

**Inchi:** InChI=1S/C27H40O2/c1-20(2)10-7-11-21(3)12-8-13-22(4)14-9-18-27(6)19-17-24-23(5)25
**InchiKey:** NWELWDHWNAURGA-NDZYPVAJSA-N
**Formula:** C27H40O2
**SMILES:** CC(C)=CCCC(C)=CCCC(C)=CCCC1(C)CCc2c(ccc(O)c2C)O1
**Mol. weight [g/mol]:** 396.61

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 287.04 | kJ/mol | Joback Method |
| hf | -292.16 | kJ/mol | Joback Method |
| hfus | 59.12 | kJ/mol | Joback Method |
| hvap | 95.87 | kJ/mol | Joback Method |
| log10ws | -9.10 | | Crippen Method |
| logp | 7.984 | | Crippen Method |
| mcvol | 355.510 | ml/mol | McGowan Method |
| pc | 1112.59 | kPa | Joback Method |
| rinpol | 3060.00 | | NIST Webbook |
| tb | 984.74 | K | Joback Method |
| tc | 1214.90 | K | Joback Method |
| tf | 565.00 | K | Joback Method |
| vc | 1.317 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1215.39 | J/mol×K | 984.74 | Joback Method |
| cpg | 1242.04 | J/mol×K | 1023.10 | Joback Method |
| cpg | 1269.54 | J/mol×K | 1061.46 | Joback Method |
| cpg | 1298.21 | J/mol×K | 1099.82 | Joback Method |
| cpg | 1328.37 | J/mol×K | 1138.18 | Joback Method |
| cpg | 1360.32 | J/mol×K | 1176.54 | Joback Method |
| cpg | 1394.38 | J/mol×K | 1214.90 | Joback Method |

# Sources

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|---|---|
| **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=R523034&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |