# «beta»-Tocopherol, O-methyl-

**Inchi:** InChI=1S/C29H50O2/c1-21(2)12-9-13-22(3)14-10-15-23(4)16-11-18-29(7)19-17-26-25(6
**InchiKey:** AGSJHGZIOXTYIA-UHFFFAOYSA-N
**Formula:** C29H50O2
**SMILES:** COc1cc(C)c2c(c1C)CCC(C)(CCCC(C)CCCC(C)CCCC(C)C)O2
**Mol. weight [g/mol]:** 430.71

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 111.91 | kJ/mol | Joback Method |
| hf | -649.42 | kJ/mol | Joback Method |
| hfus | 51.69 | kJ/mol | Joback Method |
| hvap | 89.76 | kJ/mol | Joback Method |
| log10ws | -9.86 | | Crippen Method |
| logp | 8.835 | | Crippen Method |
| mcvol | 396.590 | ml/mol | McGowan Method |
| pc | 801.15 | kPa | Joback Method |
| rinpol | 2960.00 | | NIST Webbook |
| rinpol | 2960.00 | | NIST Webbook |
| tb | 968.82 | K | Joback Method |
| tc | 1186.68 | K | Joback Method |
| tf | 535.21 | K | Joback Method |
| vc | 1.520 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1391.28 | J/mol×K | 968.82 | Joback Method |
| cpg | 1416.83 | J/mol×K | 1005.13 | Joback Method |
| cpg | 1441.82 | J/mol×K | 1041.44 | Joback Method |
| cpg | 1466.42 | J/mol×K | 1077.75 | Joback Method |
| cpg | 1490.77 | J/mol×K | 1114.06 | Joback Method |
| cpg | 1515.05 | J/mol×K | 1150.37 | Joback Method |
| cpg | 1539.41 | J/mol×K | 1186.68 | Joback Method |

# Sources

| | |
|---|---|
| **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=U374736&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

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