# (+)-«gamma»-Tocopherol, O-methyl-

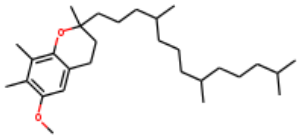
**InChI**: InChI=1S/C29H50O2/c1-21(2)12-9-13-22(3)14-10-15-23(4)16-11-18-29(7)19-17-26-20-27(30-8)24(5)25(6)28(26)31-29/h20-23H,9-19H2,1-8H3

**InChI Key**: YCYZEPRIDWTCRQ-UHFFFAOYSA-N

**Formula**: C29H50O2

**SMILES**: COc1cc2c(c(C)c1C)OC(C)(CCCC(C)CCCC(C)CCCC(C)C)CC2

**Molecular Weight**: 430.71



## Physical Properties

| Property | Value | Unit | Source |
|---|---|---|---|
| $\Delta_f G°$ | 111.91 | kJ/mol | Joback Method |
| $\Delta_f H°_{gas}$ | -649.42 | kJ/mol | Joback Method |
| $\Delta_{fus} H°$ | 51.69 | kJ/mol | Joback Method |
| $\Delta_{vap} H°$ | 89.76 | kJ/mol | Joback Method |
| $logP_{oct/wat}$ | 8.83 | | Crippen Method |
| $P_c$ | 801.15 | kPa | Joback Method |
| $T_{boil}$ | 968.82 | K | Joback Method |
| $T_c$ | 1186.68 | K | Joback Method |
| $T_{fus}$ | 535.21 | K | Joback Method |
| $V_c$ | 1.52 | $m^3$/kg-mol | Joback Method |

## Temperature Dependent Properties

| Property | Value | Unit | Temperature (K) | Source |
|---|---|---|---|---|
| $C_{p,gas}$ | 1391.28 | J/mol×K | 968.82 | Joback Method |

## Sources

**Joback Method**: https://en.wikipedia.org/wiki/Joback_method

**NIST Webbook**: http://webbook.nist.gov/cgi/inchi/InChI=1S/C29H50O2/c1-21(2)12-9-13-22(3)14-10-15-23(4)16-11-18-29(7)19-17-26-20-27(30-8)24(5)25(6)28(26)31-29/h20-23H,9-19H2,1-8H3

**Crippen Method**: http://pubs.acs.org/doi/abs/10.1021/ci990307l

## Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
$log P_{oct/wat}$: Octanol/Water partition coefficient .
$P_c$: Critical Pressure (kPa).
$T_{boil}$: Normal Boiling Point Temperature (K).
$T_c$: Critical Temperature (K).
$T_{fus}$: Normal melting (fusion) point (K).
$V_c$: Critical Volume ($m^3$/kg-mol).