# (+)-«gamma»-Tocophero, O-trifluoroacetyl-

**Inchi:** InChI=1S/C30H47F3O3/c1-20(2)11-8-12-21(3)13-9-14-22(4)15-10-17-29(7)18-16-25-19-
**InchiKey:** OWMUJRCXUOSNAV-UHFFFAOYSA-N
**Formula:** C30H47F3O3
**SMILES:** Cc1c(OC(=O)C(F)(F)F)cc2c(c1C)OC(C)(CCCC(C)CCCC(C)CCCC(C)C)CC2
**Mol. weight [g/mol]:** 512.69

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -590.18 | kJ/mol | Joback Method |
| hf | -1379.72 | kJ/mol | Joback Method |
| hfus | 57.70 | kJ/mol | Joback Method |
| hvap | 94.99 | kJ/mol | Joback Method |
| log10ws | -10.72 | | Crippen Method |
| logp | 9.294 | | Crippen Method |
| mcvol | 417.560 | ml/mol | McGowan Method |
| pc | 737.62 | kPa | Joback Method |
| rinpol | 2833.00 | | NIST Webbook |
| rinpol | 2833.00 | | NIST Webbook |
| tb | 1040.15 | K | Joback Method |
| tc | 1276.46 | K | Joback Method |
| tf | 600.60 | K | Joback Method |
| vc | 1.625 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1503.84 | J/mol×K | 1040.15 | Joback Method |
| cpg | 1530.23 | J/mol×K | 1079.54 | Joback Method |
| cpg | 1556.46 | J/mol×K | 1118.92 | Joback Method |
| cpg | 1582.79 | J/mol×K | 1158.31 | Joback Method |
| cpg | 1609.45 | J/mol×K | 1197.69 | Joback Method |
| cpg | 1636.69 | J/mol×K | 1237.08 | Joback Method |
| cpg | 1664.73 | J/mol×K | 1276.46 | 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=U374724&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 |