# (+)-«gamma»-Tocopherol, O-heptafluorobutyryl-

**Inchi:** InChI=1S/C32H47F7O3/c1-20(2)11-8-12-21(3)13-9-14-22(4)15-10-17-29(7)18-16-25-19-

**InchiKey:** XSWNWWGYYJWUBG-UHFFFAOYSA-N

**Formula:** C32H47F7O3

**SMILES:** Cc1c(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)cc2c(c1C)OC(C)(CCCC(C)CCCC(C)CCCC(C)C)C

**Mol. weight [g/mol]:** 612.70

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1346.90 | kJ/mol | Joback Method |
| hf | -2222.94 | kJ/mol | Joback Method |
| hfus | 60.37 | kJ/mol | Joback Method |
| hvap | 93.58 | kJ/mol | Joback Method |
| log10ws | -12.18 | | Crippen Method |
| logp | 10.565 | | Crippen Method |
| mcvol | 452.820 | ml/mol | McGowan Method |
| pc | 620.03 | kPa | Joback Method |
| rinpol | 2852.00 | | NIST Webbook |
| rinpol | 2852.00 | | NIST Webbook |
| tb | 1076.53 | K | Joback Method |
| tc | 1334.91 | K | Joback Method |
| tf | 630.34 | K | Joback Method |
| vc | 1.786 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1664.76 | J/mol×K | 1076.53 | Joback Method |
| cpg | 1695.11 | J/mol×K | 1119.59 | Joback Method |
| cpg | 1726.02 | J/mol×K | 1162.66 | Joback Method |
| cpg | 1757.90 | J/mol×K | 1205.72 | Joback Method |
| cpg | 1791.15 | J/mol×K | 1248.78 | Joback Method |
| cpg | 1826.17 | J/mol×K | 1291.85 | Joback Method |
| cpg | 1863.37 | J/mol×K | 1334.91 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U374726&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |