# 3-Hydroxybenzyl alcohol, bis(pentafluoropropionate)

**Inchi:** InChI=1S/C13H6F10O4/c14-10(15,12(18,19)20)8(24)26-5-6-2-1-3-7(4-6)27-9(25)11(16,1

**InchiKey:** WLTANTDSDDCSPD-UHFFFAOYSA-N

**Formula:** C13H6F10O4

**SMILES:** O=C(OCc1cccc(OC(=O)C(F)(F)C(F)(F)F)c1)C(F)(F)C(F)(F)F

**Mol. weight [g/mol]:** 416.17

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -2243.22 | kJ/mol | Joback Method |
| hf | -2572.29 | kJ/mol | Joback Method |
| hfus | 29.80 | kJ/mol | Joback Method |
| hvap | 52.43 | kJ/mol | Joback Method |
| log10ws | -5.15 | | Crippen Method |
| logp | 4.030 | | Crippen Method |
| mcvol | 202.850 | ml/mol | McGowan Method |
| pc | 1690.72 | kPa | Joback Method |
| rinpol | 1190.00 | | NIST Webbook |
| tb | 660.86 | K | Joback Method |
| tc | 833.53 | K | Joback Method |
| tf | 435.11 | K | Joback Method |
| vc | 0.840 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 580.03 | J/mol×K | 660.86 | Joback Method |
| cpg | 590.34 | J/mol×K | 689.64 | Joback Method |
| cpg | 599.82 | J/mol×K | 718.42 | Joback Method |
| cpg | 608.53 | J/mol×K | 747.20 | Joback Method |
| cpg | 616.53 | J/mol×K | 775.97 | Joback Method |
| cpg | 623.87 | J/mol×K | 804.75 | Joback Method |
| cpg | 630.59 | J/mol×K | 833.53 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U376160&Units=SI |

# 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 |