# 4-Hydroxy-3-methoxybenzyl alcohol, bis(heptafluorobutyrate)

**Inchi:** InChI=1S/C16H8F14O5/c1-33-8-4-6(5-34-9(31)11(17,18)13(21,22)15(25,26)27)2-3-7(8)3

**InchiKey:** TVNQTECLNYCNDM-UHFFFAOYSA-N

**Formula:** C16H8F14O5

**SMILES:** COc1cc(COC(=O)C(F)(F)C(F)(F)C(F)(F)F)ccc1OC(=O)C(F)(F)C(F)(F)C(F)(F)F

**Mol. weight [g/mol]:** 546.21

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -3106.15 | kJ/mol | Joback Method |
| hf | -3579.84 | kJ/mol | Joback Method |
| hfus | 35.86 | kJ/mol | Joback Method |
| hvap | 56.32 | kJ/mol | Joback Method |
| log10ws | -6.74 | | Crippen Method |
| logp | 5.310 | | Crippen Method |
| mcvol | 258.070 | ml/mol | McGowan Method |
| pc | 1194.00 | kPa | Joback Method |
| rinpol | 1426.00 | | NIST Webbook |
| tb | 747.52 | K | Joback Method |
| tc | 919.23 | K | Joback Method |
| tf | 510.87 | K | Joback Method |
| vc | 1.075 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 796.50 | J/mol×K | 747.52 | Joback Method |
| cpg | 806.53 | J/mol×K | 776.14 | Joback Method |
| cpg | 815.74 | J/mol×K | 804.76 | Joback Method |
| cpg | 824.17 | J/mol×K | 833.37 | Joback Method |
| cpg | 831.90 | J/mol×K | 861.99 | Joback Method |
| cpg | 839.00 | J/mol×K | 890.61 | Joback Method |
| cpg | 845.53 | J/mol×K | 919.23 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U376171&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

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|---|---|
| **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 |