# Homovanillic acid, acetyl, DTFMBz

**Inchi:** InChI=1S/C20H16F6O5/c1-11(27)31-16-4-3-12(7-17(16)29-2)8-18(28)30-10-13-5-14(19(
**InchiKey:** RGRLBRRFRWDYKA-UHFFFAOYSA-N
**Formula:** C20H16F6O5
**SMILES:** COc1cc(CC(=O)OCc2cc(C(F)(F)F)cc(C(F)(F)F)c2)ccc1OC(C)=O
**Mol. weight [g/mol]:** 450.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1432.20 | kJ/mol | Joback Method |
| hf | -1844.93 | kJ/mol | Joback Method |
| hfus | 44.50 | kJ/mol | Joback Method |
| hvap | 80.54 | kJ/mol | Joback Method |
| log10ws | -6.31 | | Crippen Method |
| logp | 4.944 | | Crippen Method |
| mcvol | 276.510 | ml/mol | McGowan Method |
| pc | 1378.88 | kPa | Joback Method |
| rinpol | 2108.00 | | NIST Webbook |
| rinpol | 2108.00 | | NIST Webbook |
| tb | 894.44 | K | Joback Method |
| tc | 1102.66 | K | Joback Method |
| tf | 593.01 | K | Joback Method |
| vc | 1.091 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 850.28 | J/mol×K | 894.44 | Joback Method |
| cpg | 861.41 | J/mol×K | 929.14 | Joback Method |
| cpg | 871.46 | J/mol×K | 963.85 | Joback Method |
| cpg | 880.48 | J/mol×K | 998.55 | Joback Method |
| cpg | 888.50 | J/mol×K | 1033.25 | Joback Method |
| cpg | 895.58 | J/mol×K | 1067.96 | Joback Method |
| cpg | 901.75 | J/mol×K | 1102.66 | Joback Method |

# Sources

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|---|---|
| **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=R538982&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |

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