# m-Hydroxyphenylacetic acid, TFA-ME

**Inchi:** InChI=1S/C11H9F3O4/c1-17-9(15)6-7-3-2-4-8(5-7)18-10(16)11(12,13)14/h2-5H,6H2,1H3
**InchiKey:** OQNUAMNSMLATPU-UHFFFAOYSA-N
**Formula:** C11H9F3O4
**SMILES:** COC(=O)Cc1cccc(OC(=O)C(F)(F)F)c1
**Mol. weight [g/mol]:** 262.18

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -904.91 | kJ/mol | Joback Method |
| hf | -1131.99 | kJ/mol | Joback Method |
| hfus | 25.30 | kJ/mol | Joback Method |
| hvap | 57.58 | kJ/mol | Joback Method |
| log10ws | -2.53 | | Crippen Method |
| logp | 1.870 | | Crippen Method |
| mcvol | 162.280 | ml/mol | McGowan Method |
| pc | 2545.61 | kPa | Joback Method |
| rinpol | 1275.00 | | NIST Webbook |
| tb | 629.90 | K | Joback Method |
| tc | 828.90 | K | Joback Method |
| tf | 401.18 | K | Joback Method |
| vc | 0.634 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 414.71 | J/mol×K | 629.90 | Joback Method |
| cpg | 426.13 | J/mol×K | 663.07 | Joback Method |
| cpg | 436.81 | J/mol×K | 696.23 | Joback Method |
| cpg | 446.75 | J/mol×K | 729.40 | Joback Method |
| cpg | 455.99 | J/mol×K | 762.57 | Joback Method |
| cpg | 464.53 | J/mol×K | 795.73 | Joback Method |
| cpg | 472.40 | J/mol×K | 828.90 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R387214&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 |

# 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 |