# 3,4-dihydroxymandelic acid, TFA-ME

**Inchi:** InChI=1S/C15H7F9O8/c1-29-9(25)8(32-12(28)15(22,23)24)5-2-3-6(30-10(26)13(16,17)1
**InchiKey:** JQBMUKVTPUXGJQ-UHFFFAOYSA-N
**Formula:** C15H7F9O8
**SMILES:** COC(=O)C(OC(=O)C(F)(F)F)c1ccc(OC(=O)C(F)(F)F)c(OC(=O)C(F)(F)F)c1
**Mol. weight [g/mol]:** 486.20

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -2514.32 | kJ/mol | Joback Method |
| hf | -2915.06 | kJ/mol | Joback Method |
| hfus | 40.97 | kJ/mol | Joback Method |
| hvap | 77.58 | kJ/mol | Joback Method |
| log10ws | -4.33 | | Crippen Method |
| logp | 2.942 | | Crippen Method |
| mcvol | 244.140 | ml/mol | McGowan Method |
| pc | 1583.49 | kPa | Joback Method |
| rinpol | 1370.00 | | NIST Webbook |
| rinpol | 1370.00 | | NIST Webbook |
| tb | 867.70 | K | Joback Method |
| tc | 1064.98 | K | Joback Method |
| tf | 596.48 | K | Joback Method |
| vc | 0.987 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 741.51 | J/mol×K | 867.70 | Joback Method |
| cpg | 749.26 | J/mol×K | 900.58 | Joback Method |
| cpg | 756.08 | J/mol×K | 933.46 | Joback Method |
| cpg | 762.03 | J/mol×K | 966.34 | Joback Method |
| cpg | 767.13 | J/mol×K | 999.22 | Joback Method |
| cpg | 771.41 | J/mol×K | 1032.10 | Joback Method |
| cpg | 774.91 | J/mol×K | 1064.98 | 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=R387150&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 |

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