# Sorbitol, 2-methyl, TFA

**Inchi:** InChI=1S/C17H11F15O11/c1-38-4(2-39-8(33)13(18,19)20)6(42-11(36)16(27,28)29)7(43-
**InchiKey:** MLEHIUJWCFJTTR-VZFHVOOUSA-N
**Formula:** C17H11F15O11
**SMILES:** COC(COC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(COC(=O)C(F)(F)F)OC
**Mol. weight [g/mol]:** 676.24

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -4100.05 | kJ/mol | Joback Method |
| hf | -4756.95 | kJ/mol | Joback Method |
| hfus | 49.95 | kJ/mol | Joback Method |
| hvap | 81.34 | kJ/mol | Joback Method |
| log10ws | -4.10 | | Crippen Method |
| logp | 2.635 | | Crippen Method |
| mcvol | 320.010 | ml/mol | McGowan Method |
| pc | 985.78 | kPa | Joback Method |
| rinpol | 1167.00 | | NIST Webbook |
| rinpol | 1155.00 | | NIST Webbook |
| rinpol | 1167.00 | | NIST Webbook |
| tb | 963.37 | K | Joback Method |
| tc | 1202.74 | K | Joback Method |
| tf | 625.33 | K | Joback Method |
| vc | 1.317 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1060.53 | J/mol×K | 963.37 | Joback Method |
| cpg | 1068.63 | J/mol×K | 1003.26 | Joback Method |
| cpg | 1075.19 | J/mol×K | 1043.16 | Joback Method |
| cpg | 1080.32 | J/mol×K | 1083.05 | Joback Method |
| cpg | 1084.11 | J/mol×K | 1122.95 | Joback Method |
| cpg | 1086.67 | J/mol×K | 1162.84 | Joback Method |
| cpg | 1088.10 | J/mol×K | 1202.74 | Joback Method |

# Sources

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|---|---|
| **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=R527734&Units=SI |

# 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 |