

# Sorbitol, 6-methyl, TFA

**Inchi:** InChI=1S/C17H11F15O11/c1-38-2-4(40-9(34)14(21,22)23)6(42-11(36)16(27,28)29)7(43-10(35)13(24,25)26)8(31,32)33  
**InchiKey:** YPNCBPPICCGIER-BWBBJGPYSA-N  
**Formula:** C17H11F15O11  
**SMILES:** COCC(OC(=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(F)(F)F  
**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	1115.00		NIST Webbook
rinpol	1103.00		NIST Webbook
tb	963.37	K	Joback Method
tc	1202.74	K	Joback Method
tf	625.33	K	Joback Method
vc	1.317	m <sup>3</sup> /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

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R527823&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R527823&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>h vap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r in pol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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