

# Sorbitol, 2,3,6-trimethyl, TFA

**Inchi:** InChI=1S/C15H17F9O9/c1-28-4-7(32-11(26)14(19,20)21)9(33-12(27)15(22,23)24)8(30-3  
**InchiKey:** JBIRWIOENMLNLD-KZVJFYERSA-N  
**Formula:** C15H17F9O9  
**SMILES:** COCC(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC)C(COC(=O)C(F)(F)F)OC  
**Mol. weight [g/mol]:** 512.28

## Physical Properties

Property code	Value	Unit	Source
gf	-2695.87	kJ/mol	Joback Method
hf	-3296.35	kJ/mol	Joback Method
hfus	37.92	kJ/mol	Joback Method
hvap	70.89	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	1.717		Crippen Method
mcvol	278.070	ml/mol	McGowan Method
pc	1199.79	kPa	Joback Method
rinpol	1335.00		NIST Webbook
rinpol	1327.00		NIST Webbook
tb	820.71	K	Joback Method
tc	1004.78	K	Joback Method
tf	494.55	K	Joback Method
vc	1.107	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	887.11	J/molxK	820.71	Joback Method
cpg	898.89	J/molxK	851.39	Joback Method
cpg	909.62	J/molxK	882.07	Joback Method
cpg	919.33	J/molxK	912.75	Joback Method
cpg	928.03	J/molxK	943.43	Joback Method
cpg	935.72	J/molxK	974.11	Joback Method
cpg	942.42	J/molxK	1004.78	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R527645&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R527645&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>hvpap:</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>rinppl:</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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