

# Adonitol, pentakis(trifluoroacetate)

<b>Inchi:</b>	InChI=1S/C15H7F15O10/c16-11(17,18)6(31)36-1-3(38-8(33)13(22,23)24)5(40-10(35)15
<b>InchiKey:</b>	VKRTZHFVBRDDBC-UHFFFAOYSA-N
<b>Formula:</b>	C15H7F15O10
<b>SMILES:</b>	O=C(OCC(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(COC(=O)C(F)(F)F)OC(=O)C(F)(F)F)C
<b>Mol. weight [g/mol]:</b>	632.19

## Physical Properties

Property code	Value	Unit	Source
gf	-4009.45	kJ/mol	Joback Method
hf	-4578.17	kJ/mol	Joback Method
hfus	47.10	kJ/mol	Joback Method
hvap	74.86	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	2.620		Crippen Method
mvol	285.960	ml/mol	McGowan Method
pc	1123.06	kPa	Joback Method
rinpol	1039.20		NIST Webbook
rinpol	1039.20		NIST Webbook
tb	895.63	K	Joback Method
tc	1104.84	K	Joback Method
tf	595.56	K	Joback Method
vc	1.192	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	925.57	J/molxK	895.63	Joback Method
cpg	933.39	J/molxK	930.50	Joback Method
cpg	940.12	J/molxK	965.37	Joback Method
cpg	945.84	J/molxK	1000.23	Joback Method
cpg	950.61	J/molxK	1035.10	Joback Method
cpg	954.51	J/molxK	1069.97	Joback Method
cpg	957.62	J/molxK	1104.84	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U380207&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380207&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>hvap:</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>rinpolar:</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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