

# D-(-)-Fructofuranose, pentakis(trifluoroacetate) (isomer 1)

<b>Inchi:</b>	InChI=1S/C16H7F15O11/c17-12(18,19)6(32)37-1-3-4(39-8(34)14(23,24)25)5(40-9(35)15
<b>InchiKey:</b>	XZVKUTGQYBCICM-UHFFFAOYSA-N
<b>Formula:</b>	C16H7F15O11
<b>SMILES:</b>	O=C(OCC1OC(COC(=O)C(F)(F)F)(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C1OC(=O)C(F)
<b>Mol. weight [g/mol]:</b>	660.20

## Physical Properties

Property code	Value	Unit	Source
gf	-4071.90	kJ/mol	Joback Method
hf	-4700.27	kJ/mol	Joback Method
hfus	59.09	kJ/mol	Joback Method
hvap	80.94	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	2.346		Crippen Method
mcvol	295.060	ml/mol	McGowan Method
pc	1120.80	kPa	Joback Method
rinpol	1146.70		NIST Webbook
rinpol	1146.70		NIST Webbook
tb	948.29	K	Joback Method
tc	1170.12	K	Joback Method
tf	700.48	K	Joback Method
vc	1.224	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1010.35	J/molxK	948.29	Joback Method
cpg	1021.57	J/molxK	985.26	Joback Method
cpg	1032.33	J/molxK	1022.23	Joback Method
cpg	1042.81	J/molxK	1059.20	Joback Method
cpg	1053.18	J/molxK	1096.18	Joback Method
cpg	1063.59	J/molxK	1133.15	Joback Method
cpg	1074.22	J/molxK	1170.12	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U380306&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380306&amp;Units=SI</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>hvp:</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>rinp:</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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