

# L-(-)-Fucopyranose, tetrakis(trifluoroacetate) (isomer 1)

<b>Inchi:</b>	InChI=1S/C14H8F12O9/c1-2-3(32-7(27)11(15,16)17)4(33-8(28)12(18,19)20)5(34-9(29)1
<b>InchiKey:</b>	QCBFFHJNJFCVIR-UHFFFAOYSA-N
<b>Formula:</b>	C14H8F12O9
<b>SMILES:</b>	CC1OC(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C1OC(=O)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	548.19

## Physical Properties

Property code	Value	Unit	Source
gf	-3287.55	kJ/mol	Joback Method
hf	-3858.85	kJ/mol	Joback Method
hfus	54.57	kJ/mol	Joback Method
hvap	72.10	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	2.259		Crippen Method
mcvol	254.130	ml/mol	McGowan Method
pc	1295.79	kPa	Joback Method
rinsol	1033.00		NIST Webbook
tb	831.02	K	Joback Method
tc	1017.82	K	Joback Method
tf	569.93	K	Joback Method
vc	1.038	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.28	J/molxK	831.02	Joback Method
cpg	861.50	J/molxK	862.15	Joback Method
cpg	870.60	J/molxK	893.29	Joback Method
cpg	878.60	J/molxK	924.42	Joback Method
cpg	885.54	J/molxK	955.56	Joback Method
cpg	891.42	J/molxK	986.69	Joback Method
cpg	896.30	J/molxK	1017.82	Joback Method

# Sources

<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>
<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=U380259&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380259&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>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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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