

L-(-)-Fucopyranose, tetrakis(trifluoroacetate) (isomer 2)

Inchi:	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
InchiKey:	QCBFFHJNJFCVIR-UHFFFAOYSA-N
Formula:	C14H8F12O9
SMILES:	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
Mol. weight [g/mol]:	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
rinpol	1116.00		NIST Webbook
tb	831.02	K	Joback Method
tc	1017.82	K	Joback Method
tf	569.93	K	Joback Method
vc	1.038	m3/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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380262&Units=SI

Legend

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

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