L-(-)-Fucofuranose, tetrakis(trifluoroacetate) (isomer 1)

Inchi: InChI=1S/C14H8F12O9/c1-2(31-7(27)11(15,16)17)3-4(33-8(28)12(18,19)20)5(34-9(29)1
InchiKey: MHTQWNCTUKUZAN-UHFFFAOYSA-N
Formula: C14H8F12O9
SMILES: CC(OC(=O)C(F)(F)F)C1OC(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	-3270.18	kJ/mol	Joback Method
hf	-3837.63	kJ/mol	Joback Method
hfus	52.07	kJ/mol	Joback Method
hvap	71.85	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	2.259		Crippen Method
mcvol	254.130	ml/mol	McGowan Method
pc	1310.85	kPa	Joback Method
rinpol	1065.40		NIST Webbook
tb	830.98	K	Joback Method
tc	1017.60	K	Joback Method
tf	562.69	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	844.21	J/mol×K	830.98	Joback Method
cpg	854.05	J/mol×K	862.08	Joback Method
cpg	862.86	J/mol×K	893.19	Joback Method
cpg	870.67	J/mol×K	924.29	Joback Method
cpg	877.52	J/mol×K	955.40	Joback Method
cpg	883.44	J/mol×K	986.50	Joback Method
cpg	888.47	J/mol×K	1017.60	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=U380263&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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