D-(+)-Xylofuranose, tetrakis(trifluoroacetate) (isomer 1)

Inchi: InChI=1S/C13H6F12O9/c14-10(15,16)6(26)30-1-2-3(32-7(27)11(17,18)19)4(33-8(28)12(
InchiKey: XEYHCBFOSDMJES-UHFFFAOYSA-N
Formula: C13H6F12O9
SMILES: O=C(OCC1OC(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C1OC(=O)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 534.16

Physical Properties

Property code	Value	Unit	Source
gf	-3276.16	kJ/mol	Joback Method
hf	-3811.71	kJ/mol	Joback Method
hfus	53.01	kJ/mol	Joback Method
hvap	70.01	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	1.871		Crippen Method
mcvol	240.040	ml/mol	McGowan Method
pc	1398.55	kPa	Joback Method
rinpol	1123.00		NIST Webbook
rinpol	1123.00		NIST Webbook
tb	808.54	K	Joback Method
tc	990.69	K	Joback Method
tf	566.42	K	Joback Method
vc	0.991	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	789.07	J/mol×K	808.54	Joback Method
cpg	798.55	J/mol×K	838.90	Joback Method
cpg	807.08	J/mol×K	869.26	Joback Method
cpg	814.67	J/mol×K	899.61	Joback Method
cpg	821.38	J/mol×K	929.97	Joback Method
cpg	827.22	J/mol×K	960.33	Joback Method
cpg	832.23	J/mol×K	990.69	Joback Method

Sources

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=U380290&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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