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

Inchi: InChI=1S/C13H6F12O9/c14-10(15,16)6(26)31-2-1-30-5(34-9(29)13(23,24)25)4(33-8(28)
InchiKey: ZHQMHGFJNVQNHH-UHFFFAOYSA-N
Formula: C13H6F12O9
SMILES: O=C(OC1COC(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	-3288.26	kJ/mol	Joback Method
hf	-3817.87	kJ/mol	Joback Method
hfus	50.91	kJ/mol	Joback Method
hvap	70.18	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	1.871		Crippen Method
mcvol	240.040	ml/mol	McGowan Method
pc	1425.07	kPa	Joback Method
rinpol	1043.20		NIST Webbook
rinpol	1043.20		NIST Webbook
tb	812.81	K	Joback Method
tc	996.58	K	Joback Method
tf	562.90	K	Joback Method
vc	0.983	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.14	J/mol×K	812.81	Joback Method
cpg	801.74	J/mol×K	843.44	Joback Method
cpg	810.31	J/mol×K	874.07	Joback Method
cpg	817.89	J/mol×K	904.69	Joback Method
cpg	824.49	J/mol×K	935.32	Joback Method
cpg	830.16	J/mol×K	965.95	Joback Method
cpg	834.91	J/mol×K	996.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380288&Units=SI
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

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