D-(+)-Xylose, tetrakis(trifluoroacetate), methyloxime (anti)

Inchi: InChI=1S/C14H9F12NO9/c1-32-27-2-4(34-8(29)12(18,19)20)6(36-10(31)14(24,25)26)5(3

InchiKey: BOAISAABNRWOGO-UHFFFAOYSA-N

Formula: C14H9F12NO9

SMILES: CON=CC(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(COC(=O)C(F)(F)F)OC(=O)C(F)(F)F

Mol. weight [g/mol]: 563.20

Physical Properties

Property code	Value	Unit	Source
hf	-3765.65	kJ/mol	Joback Method
hvap	72.95	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	2.146		Crippen Method
mcvol	270.670	ml/mol	McGowan Method
pc	1156.93	kPa	Joback Method
rinpol	1103.20		NIST Webbook
rinpol	1103.20		NIST Webbook
tb	900.98	K	Joback Method
tc	1104.62	K	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=U380231&Units=SI

Legend

hf: Enthalpy of formation 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

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