N-Acetyl-D-glucosamine, tetrakis(trifluoroacetate), methyloxime (syn)

Inchi: InChI=1S/C17H14F12N2O10/c1-5(32)31-6(3-30-37-2)8(40-12(35)16(24,25)26)9(41-13(3

InchiKey: JPSFBHXVCJIGTG-UHFFFAOYSA-N

Formula: C17H14F12N2O10

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

Mol. weight [g/mol]: 634.28

Physical Properties

Property code	Value	Unit	Source
hf	-3891.96	kJ/mol	Joback Method
hvap	92.43	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	1.651		Crippen Method
mcvol	324.490	ml/mol	McGowan Method
pc	1011.66	kPa	Joback Method
rinpol	1451.40		NIST Webbook
rinpol	1451.40		NIST Webbook
tb	1073.22	K	Joback Method
tc	1342.61	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U380243&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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