L-(-)-Fucose, tetrakis(trifluoroacetate), benzyloxime (isomer 1)

Inchi: InChI=1S/C21H15F12NO9/c1-9(40-14(35)18(22,23)24)12(42-16(37)20(28,29)30)13(43-1

InchiKey: NADUNPKOYVTNSH-UHFFFAOYSA-N

Formula: C21H15F12NO9

SMILES: CC(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(C=NOCc1ccccc1)OC(=O

Mol. weight [g/mol]: 653.33

Physical Properties

Property code	Value	Unit	Source
hf	-3678.88	kJ/mol	Joback Method
hvap	90.42	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	4.105		Crippen Method
mcvol	345.540	ml/mol	McGowan Method
pc	933.49	kPa	Joback Method
rinpol	1889.30		NIST Webbook
tb	1087.38	K	Joback Method
tc	1349.76	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=U380452&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