2-Deoxy-D-ribose, tris(trifluoroacetate), methyloxime (isomer 1)

Inchi: InChI=1S/C12H10F9NO7/c1-26-22-3-2-5(28-8(24)11(16,17)18)6(29-9(25)12(19,20)21)4-

InchiKey: VKXDKGHDCPATCL-UHFFFAOYSA-N

Formula: C12H10F9NO7

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

Mol. weight [g/mol]: 451.20

Physical Properties

Property code	Value	Unit	Source
hf	-2877.21	kJ/mol	Joback Method
hvap	63.48	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.062		Crippen Method
mcvol	229.740	ml/mol	McGowan Method
pc	1386.08	kPa	Joback Method
rinpol	1138.80		NIST Webbook
rinpol	1138.80		NIST Webbook
tb	784.79	K	Joback Method
tc	964.80	K	Joback Method

Sources

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=U380249&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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