1-Chloro-1-deoxyfructose, tetrakis(trifluoroacetate), methyloxime

Inchi: InChI=1S/C15H10ClF12NO9/c1-34-29-4(2-16)6(37-10(32)14(23,24)25)7(38-11(33)15(26

InchiKey: FCKRVLAPGXEFND-UHFFFAOYSA-N

Formula: C15H10ClF12NO9

SMILES: CON=C(CCl)C(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

Mol. weight [g/mol]: 611.67

Physical Properties

Property code	Value	Unit	Source
hf	-3811.82	kJ/mol	Joback Method
hvap	79.64	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	2.755		Crippen Method
mcvol	297.000	ml/mol	McGowan Method
pc	1062.40	kPa	Joback Method
rinpol	1235.30		NIST Webbook
rinpol	1235.30		NIST Webbook
tb	961.17	K	Joback Method
tc	1182.36	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=U380285&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