

L-(-)-Fucose, tetrakis(trifluoroacetate), methyloxime (anti)

Inchi: InChI=1S/C15H11F12NO9/c1-4(34-8(29)12(16,17)18)6(36-10(31)14(22,23)24)7(37-11(32)13)5(33)2
InchiKey: ZLROHNZHWFCGJA-UHFFFAOYSA-N
Formula: C15H11F12NO9
SMILES: CON=CC(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(C)OC(=O)C(F)(F)F
Mol. weight [g/mol]: 577.23

Physical Properties

Property code	Value	Unit	Source
hf	-3791.57	kJ/mol	Joback Method
hvap	74.79	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	2.535		Crippen Method
mcvol	284.760	ml/mol	McGowan Method
pc	1090.66	kPa	Joback Method
rinsol	1070.50		NIST Webbook
tb	923.42	K	Joback Method
tc	1133.42	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=U380223&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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