D-(+)-Mannose, pentakis(trifluoroacetate), methyloxime (syn)

Inchi: InChI=1S/C17H10F15NO11/c1-39-33-2-4(41-9(35)14(21,22)23)6(43-11(37)16(27,28)29)
InchiKey: IOALWQFXAPVULK-UHFFFAOYSA-N
Formula: C17H10F15NO11
SMILES: CON=CC(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(COC(=O)C(F)(F)F
Mol. weight [g/mol]: 689.24

Physical Properties

Property code	Value	Unit	Source
hf	-4674.73	kJ/mol	Joback Method
hvap	84.65	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	2.620		Crippen Method
mcvol	325.690	ml/mol	McGowan Method
pc	923.86	kPa	Joback Method
rinpol	1164.90		NIST Webbook
rinpol	1164.90		NIST Webbook
tb	1040.05	K	Joback Method
tc	1307.10	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U380230&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

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