D-(-)-Fructose, pentaacetate, benzyloxime (isomer 2)

Inchi: InChI=1S/C23H29NO11/c1-14(25)30-12-20(24-32-11-19-9-7-6-8-10-19)22(34-17(4)28)23

InchiKey: SAWPFTSVIQTCGL-UHFFFAOYSA-N

Formula: C23H29NO11

SMILES: CC(=O)OCC(=NOCc1ccccc1)C(OC(C)=O)C(OC(C)=O)C(COC(C)=O)OC(C)=O

Mol. weight [g/mol]: 495.48

Physical Properties

Property code	Value	Unit	Source
hf	-1581.15	kJ/mol	Joback Method
hvap	119.49	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	1.480		Crippen Method
mcvol	359.920	ml/mol	McGowan Method
pc	1142.89	kPa	Joback Method
rinpol	2608.90		NIST Webbook
rinpol	2608.90		NIST Webbook
tb	1231.43	K	Joback Method
tc	1518.70	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U380446&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

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