

D-(-)-Fructose, pentaacetate, benzyloxime (isomer 1)

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:	SAWPFTSVIQTGCL-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	2578.60		NIST Webbook
tb	1231.43	K	Joback Method
tc	1518.70	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380445&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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