

L-(-)-Fucose, tetraacetate, benzylloxime (isomer 1)

Inchi:	InChI=1S/C21H27NO9/c1-13(28-14(2)23)20(30-16(4)25)21(31-17(5)26)19(29-15(3)24)1
InchiKey:	LJCRDKAZVRSCFU-UHFFFAOYSA-N
Formula:	C21H27NO9
SMILES:	CC(=O)OC(C)C(OC(C)=O)C(OC(C)=O)C(C=NOCc1ccccc1)OC(C)=O
Mol. weight [g/mol]:	437.44

Physical Properties

Property code	Value	Unit	Source
hf	-1290.56	kJ/mol	Joback Method
hvap	105.41	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	1.936		Crippen Method
mcvol	324.300	ml/mol	McGowan Method
pc	1267.35	kPa	Joback Method
rinpol	2323.80		NIST Webbook
rinpol	2323.80		NIST Webbook
tb	1109.06	K	Joback Method
tc	1357.81	K	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U380449&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

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