L-(+)-Erythrulose, acetyloxime, triacetate (isomer 2)

Inchi: InChI=1S/C12H17NO8/c1-7(14)18-5-11(13-21-10(4)17)12(20-9(3)16)6-19-8(2)15/h12H,5

InchiKey: QOONVROLOPCEGM-UHFFFAOYSA-N

Formula: C12H17NO8

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

Mol. weight [g/mol]: 303.27

Physical Properties

Property code	Value	Unit	Source
hf	-1203.06	kJ/mol	Joback Method
hvap	81.94	kJ/mol	Joback Method
log10ws	-0.56		Crippen Method
logp	-0.037		Crippen Method
mcvol	215.380	ml/mol	McGowan Method
pc	1927.05	kPa	Joback Method
rinpol	1803.70		NIST Webbook
rinpol	1803.70		NIST Webbook
tb	855.24	K	Joback Method
tc	1064.44	K	Joback Method

Sources

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=U380436&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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