2,3,5-Tri-O-Acetyl-1,4-Anhydro-L-fucitol

Inchi: InChI=1S/C12H18O7/c1-6(17-7(2)13)11-12(19-9(4)15)10(5-16-11)18-8(3)14/h6,10-12H,5
InchiKey: SSTYJVAQXLVKEY-KNFQTBNASA-N
Formula: C12H18O7
SMILES: CC(=O)OC(C)C1OCC(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]: 274.27

Physical Properties

Property code	Value	Unit	Source
gf	-719.03	kJ/mol	Joback Method
hf	-1142.89	kJ/mol	Joback Method
hfus	35.73	kJ/mol	Joback Method
hvap	73.53	kJ/mol	Joback Method
log10ws	-0.86		Crippen Method
logp	0.200		Crippen Method
mcvol	197.270	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
rinpol	1617.58		NIST Webbook
rinpol	1617.58		NIST Webbook
tb	735.28	K	Joback Method
tc	941.31	K	Joback Method
tf	455.47	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.41	J/mol×K	735.28	Joback Method
cpg	605.37	J/mol×K	769.62	Joback Method
cpg	619.29	J/mol×K	803.96	Joback Method
cpg	632.14	J/mol×K	838.30	Joback Method
cpg	643.90	J/mol×K	872.63	Joback Method
cpg	654.55	J/mol×K	906.97	Joback Method
cpg	664.06	J/mol×K	941.31	Joback Method
dvisc	0.0013646	Pa×s	455.47	Joback Method

dvisc	0.0008668	Pa×s	502.11	Joback Method
dvisc	0.0005947	Pa×s	548.74	Joback Method
dvisc	0.0004329	Pa×s	595.38	Joback Method
dvisc	0.0003299	Pa×s	642.01	Joback Method
dvisc	0.0002609	Pa×s	688.64	Joback Method
dvisc	0.0002126	Pa×s	735.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R180771&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

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume