2,3-di-O-acetyl-1,4-anhydro-4-O-methyl-D-fucitol

Inchi: InChI=1S/C11H18O6/c1-6-10(14-4)11(17-8(3)13)9(5-15-6)16-7(2)12/h6,9-11H,5H2,1-4H
InchiKey: BMQHDPCUPLQPJZ-UHFFFAOYSA-N
Formula: C11H18O6
SMILES: COC1C(C)OCC(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]: 246.26

Physical Properties

Property code	Value	Unit	Source
gf	-615.90	kJ/mol	Joback Method
hf	-1030.89	kJ/mol	Joback Method
hfus	34.03	kJ/mol	Joback Method
hvap	64.81	kJ/mol	Joback Method
log10ws	-0.67		Crippen Method
logp	0.283		Crippen Method
mcvol	181.610	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
rinpol	1515.80		NIST Webbook
rinpol	1515.80		NIST Webbook
tb	658.57	K	Joback Method
tc	862.68	K	Joback Method
tf	401.51	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.31	J/mol×K	658.57	Joback Method
cpg	538.33	J/mol×K	692.59	Joback Method
cpg	554.40	J/mol×K	726.61	Joback Method
cpg	569.49	J/mol×K	760.63	Joback Method
cpg	583.56	J/mol×K	794.64	Joback Method
cpg	596.58	J/mol×K	828.66	Joback Method
cpg	608.52	J/mol×K	862.68	Joback Method
dvisc	0.0012794	Pa×s	401.51	Joback Method

dvisc	0.0008278	Pa×s	444.35	Joback Method
dvisc	0.0005783	Pa×s	487.20	Joback Method
dvisc	0.0004281	Pa×s	530.04	Joback Method
dvisc	0.0003314	Pa×s	572.88	Joback Method
dvisc	0.0002659	Pa×s	615.73	Joback Method
dvisc	0.0002196	Pa×s	658.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R221624&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