2,5-Di-O-acetyl-1,4-anhydro-3-O-methyl-L-fucitol

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

Physical Properties

Property code	Value	Unit	Source
gf	-598.53	kJ/mol	Joback Method
hf	-1009.67	kJ/mol	Joback Method
hfus	31.54	kJ/mol	Joback Method
hvap	64.56	kJ/mol	Joback Method
log10ws	-0.67		Crippen Method
logp	0.283		Crippen Method
mcvol	181.610	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
rinpol	1492.78		NIST Webbook
rinpol	1492.78		NIST Webbook
tb	658.53	K	Joback Method
tc	860.46	K	Joback Method
tf	394.27	K	Joback Method
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.37	J/mol×K	658.53	Joback Method
cpg	588.90	J/mol×K	826.81	Joback Method
cpg	576.46	J/mol×K	793.15	Joback Method
cpg	563.07	J/mol×K	759.50	Joback Method
cpg	548.74	J/mol×K	725.84	Joback Method
cpg	533.50	J/mol×K	692.19	Joback Method
cpg	600.36	J/mol×K	860.46	Joback Method
dvisc	0.0002298	Pa×s	658.53	Joback Method

dvisc	0.0002822	Pa×s	614.49	Joback Method
dvisc	0.0003576	Pa×s	570.44	Joback Method
dvisc	0.0004715	Pa×s	526.40	Joback Method
dvisc	0.0006539	Pa×s	482.36	Joback Method
dvisc	0.0009684	Pa×s	438.31	Joback Method
dvisc	0.0015656	Pa×s	394.27	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357239&Units=SI

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

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