5-O-Acetyl-1,4-anhydro-2,3-di-O-methyl-L-fucitol

Inchi: InChI=1S/C10H18O5/c1-6(15-7(2)11)9-10(13-4)8(12-3)5-14-9/h6,8-10H,5H2,1-4H3
InchiKey: DOZOQRIDOIDCSF-UHFFFAOYSA-N
Formula: C10H18O5
SMILES: COC1COC(C(C)OC(C)=O)C1OC
Mol. weight [g/mol]: 218.25

Physical Properties

Property code	Value	Unit	Source
gf	-478.03	kJ/mol	Joback Method
hf	-876.45	kJ/mol	Joback Method
hfus	27.35	kJ/mol	Joback Method
hvap	55.59	kJ/mol	Joback Method
log10ws	-0.47		Crippen Method
logp	0.367		Crippen Method
mcvol	165.950	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
rinpol	1372.13		NIST Webbook
tb	581.78	K	Joback Method
tc	779.20	K	Joback Method
tf	333.07	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.42	J/mol×K	581.78	Joback Method
cpg	519.81	J/mol×K	746.30	Joback Method
cpg	506.10	J/mol×K	713.40	Joback Method
cpg	491.58	J/mol×K	680.49	Joback Method
cpg	476.29	J/mol×K	647.59	Joback Method
cpg	460.23	J/mol×K	614.68	Joback Method
cpg	532.69	J/mol×K	779.20	Joback Method
dvisc	0.0002349	Pa×s	581.78	Joback Method
dvisc	0.0002880	Pa×s	540.33	Joback Method

dvisc	0.0003652	Pa×s	498.88	Joback Method
dvisc	0.0004835	Pa×s	457.42	Joback Method
dvisc	0.0006770	Pa×s	415.97	Joback Method
dvisc	0.0010211	Pa×s	374.52	Joback Method
dvisc	0.0017061	Pa×s	333.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357237&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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