2-O-acetyl-1,5-anhydro-3,4-di-O-methyl-D-fucitol

Inchi: InChI=1S/C10H18O5/c1-6-9(12-3)10(13-4)8(5-14-6)15-7(2)11/h6,8-10H,5H2,1-4H3
InchiKey: IOZKBHQZAGQIFL-UHFFFAOYSA-N
Formula: C10H18O5
SMILES: COC1C(C)OCC(OC(C)=O)C1OC
Mol. weight [g/mol]: 218.25

Physical Properties

Property code	Value	Unit	Source
gf	-495.40	kJ/mol	Joback Method
hf	-897.67	kJ/mol	Joback Method
hfus	29.85	kJ/mol	Joback Method
hvap	55.84	kJ/mol	Joback Method
log10ws	-0.47		Crippen Method
logp	0.367		Crippen Method
mcvol	165.950	ml/mol	McGowan Method
pc	2336.03	kPa	Joback Method
rinpol	1419.35		NIST Webbook
tb	581.82	K	Joback Method
tc	781.60	K	Joback Method
tf	340.31	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.71	J/mol×K	581.82	Joback Method
cpg	463.43	J/mol×K	615.12	Joback Method
cpg	480.39	J/mol×K	648.41	Joback Method
cpg	496.55	J/mol×K	681.71	Joback Method
cpg	511.88	J/mol×K	715.01	Joback Method
cpg	526.35	J/mol×K	748.31	Joback Method
cpg	539.92	J/mol×K	781.60	Joback Method
dvisc	0.0013331	Pa×s	340.31	Joback Method
dvisc	0.0008435	Pa×s	380.56	Joback Method

dvisc	0.0005826	Pa×s	420.81	Joback Method
dvisc	0.0004292	Pa×s	461.06	Joback Method
dvisc	0.0003321	Pa×s	501.32	Joback Method
dvisc	0.0002670	Pa×s	541.57	Joback Method
dvisc	0.0002212	Pa×s	581.82	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=R221644&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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