3-O-acetyl-1,5-Anhydro-2,4-di-O-methyl-D-ribitol

Inchi: InChI=1S/C9H16O5/c1-6(10)14-9-7(11-2)4-13-5-8(9)12-3/h7-9H,4-5H2,1-3H3/t7-,8+,9-
InchiKey: QTOOMCJAZKKGNQ-AYMMMOKOSA-N
Formula: C9H16O5
SMILES: COC1COCC(OC)C1OC(C)=O
Mol. weight [g/mol]: 204.22

Physical Properties

Property code	Value	Unit	Source
gf	-496.11	kJ/mol	Joback Method
hf	-856.69	kJ/mol	Joback Method
hfus	26.19	kJ/mol	Joback Method
hvap	53.92	kJ/mol	Joback Method
log10ws	0.06		Crippen Method
logp	-0.022		Crippen Method
mcvol	151.860	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
rinpol	1308.86		NIST Webbook
rinpol	1308.86		NIST Webbook
tb	563.61	K	Joback Method
tc	766.45	K	Joback Method
tf	333.28	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.65	J/mol×K	563.61	Joback Method
cpg	411.26	J/mol×K	597.42	Joback Method
cpg	427.15	J/mol×K	631.22	Joback Method
cpg	442.31	J/mol×K	665.03	Joback Method
cpg	456.70	J/mol×K	698.84	Joback Method
cpg	470.29	J/mol×K	732.64	Joback Method
cpg	483.06	J/mol×K	766.45	Joback Method
dvisc	0.0015574	Pa×s	333.28	Joback Method

dvisc	0.0009409	Pa×s	371.67	Joback Method
dvisc	0.0006247	Pa×s	410.06	Joback Method
dvisc	0.0004449	Pa×s	448.44	Joback Method
dvisc	0.0003342	Pa×s	486.83	Joback Method
dvisc	0.0002618	Pa×s	525.22	Joback Method
dvisc	0.0002121	Pa×s	563.61	Joback Method

Sources

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=R194631&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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