5-O-Acetyl-1,4-anhydro-2,3-di-O-methyl-D-ribitol

Other names: 5-O-Acetyl-1,4-Anhydro-2,3-di-O-methyl-D-xylitol
Inchi: InChI=1S/C9H16O5/c1-6(10)13-5-8-9(12-3)7(11-2)4-14-8/h7-9H,4-5H2,1-3H3
InchiKey: ZUPAPOIBLPNRRS-UHFFFAOYSA-N
Formula: C9H16O5
SMILES: COC1COC(COC(C)=O)C1OC
Mol. weight [g/mol]: 204.22

Physical Properties

Property code	Value	Unit	Source
gf	-484.01	kJ/mol	Joback Method
hf	-850.53	kJ/mol	Joback Method
hfus	28.29	kJ/mol	Joback Method
hvap	53.75	kJ/mol	Joback Method
log10ws	0.06		Crippen Method
logp	-0.022		Crippen Method
mcvol	151.860	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
rinpol	1397.87		NIST Webbook
rinpol	1397.87		NIST Webbook
tb	559.34	K	Joback Method
tc	755.50	K	Joback Method
tf	336.80	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.71	J/mol×K	559.34	Joback Method
cpg	409.40	J/mol×K	592.03	Joback Method
cpg	424.45	J/mol×K	624.73	Joback Method
cpg	438.84	J/mol×K	657.42	Joback Method
cpg	452.54	J/mol×K	690.12	Joback Method
cpg	465.53	J/mol×K	722.81	Joback Method
cpg	477.80	J/mol×K	755.50	Joback Method

dvisc	0.0014298	Pa×s	336.80	Joback Method
dvisc	0.0009431	Pa×s	373.89	Joback Method
dvisc	0.0006706	Pa×s	410.98	Joback Method
dvisc	0.0005045	Pa×s	448.07	Joback Method
dvisc	0.0003965	Pa×s	485.16	Joback Method
dvisc	0.0003224	Pa×s	522.25	Joback Method
dvisc	0.0002695	Pa×s	559.34	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=U357229&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