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

Inchi: InChI=1S/C9H18O4/c1-6-8(11-3)9(12-4)7(10-2)5-13-6/h6-9H,5H2,1-4H3
InchiKey: VOHHBIXLBGOYCN-UHFFFAOYSA-N
Formula: C9H18O4
SMILES: COC1COC(C)C(OC)C1OC
Mol. weight [g/mol]: 190.24

Physical Properties

Property code	Value	Unit	Source
gf	-374.90	kJ/mol	Joback Method
hf	-764.45	kJ/mol	Joback Method
hfus	25.66	kJ/mol	Joback Method
hvap	46.87	kJ/mol	Joback Method
log10ws	-0.28		Crippen Method
logp	0.450		Crippen Method
mcvol	150.290	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
rinpol	1226.52		NIST Webbook
rinpol	1226.52		NIST Webbook
tb	505.07	K	Joback Method
tc	699.06	K	Joback Method
tf	279.11	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.57	J/mol×K	505.07	Joback Method
cpg	453.28	J/mol×K	666.73	Joback Method
cpg	438.03	J/mol×K	634.40	Joback Method
cpg	422.10	J/mol×K	602.07	Joback Method
cpg	405.53	J/mol×K	569.73	Joback Method
cpg	388.34	J/mol×K	537.40	Joback Method
cpg	467.83	J/mol×K	699.06	Joback Method
dvisc	0.0002049	Pa×s	505.07	Joback Method

dvisc	0.0002455	Pa×s	467.41	Joback Method
dvisc	0.0003035	Pa×s	429.75	Joback Method
dvisc	0.0003909	Pa×s	392.09	Joback Method
dvisc	0.0005313	Pa×s	354.43	Joback Method
dvisc	0.0007767	Pa×s	316.77	Joback Method
dvisc	0.0012581	Pa×s	279.11	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=R221604&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