1,4-Anhydro-2,3,5-tri-O-methyl-L-fucitol

Inchi: InChI=1S/C9H18O4/c1-6(10-2)8-9(12-4)7(11-3)5-13-8/h6-9H,5H2,1-4H3
InchiKey: VYYXUPGWUOGQQX-UHFFFAOYSA-N
Formula: C9H18O4
SMILES: COC(C)C1OCC(OC)C1OC
Mol. weight [g/mol]: 190.24

Physical Properties

Property code	Value	Unit	Source
gf	-357.53	kJ/mol	Joback Method
hf	-743.23	kJ/mol	Joback Method
hfus	23.16	kJ/mol	Joback Method
hvap	46.62	kJ/mol	Joback Method
log10ws	-0.28		Crippen Method
logp	0.450		Crippen Method
mcvol	150.290	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	1229.98		NIST Webbook
rinpol	1229.98		NIST Webbook
tb	505.03	K	Joback Method
tc	696.54	K	Joback Method
tf	271.87	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.90	J/mol×K	505.03	Joback Method
cpg	448.25	J/mol×K	664.62	Joback Method
cpg	433.84	J/mol×K	632.70	Joback Method
cpg	418.78	J/mol×K	600.78	Joback Method
cpg	403.09	J/mol×K	568.87	Joback Method
cpg	386.79	J/mol×K	536.95	Joback Method
cpg	462.00	J/mol×K	696.54	Joback Method
dvisc	0.0002217	Pa×s	505.03	Joback Method

dvisc	0.0002705	Pa×s	466.17	Joback Method
dvisc	0.0003422	Pa×s	427.31	Joback Method
dvisc	0.0004536	Pa×s	388.45	Joback Method
dvisc	0.0006402	Pa×s	349.59	Joback Method
dvisc	0.0009851	Pa×s	310.73	Joback Method
dvisc	0.0017142	Pa×s	271.87	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=U412116&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