1,5-Anhydro-4,6-di-O-acetyl-2,3-di-O-methyl-D-glu

Other names: 4,6-di-O-Acetyl-1,5-anhydro-2,3-di-O-methyl-D-glucitol
Inchi: InChI=1S/C12H20O7/c1-7(13)17-6-10-12(19-8(2)14)11(16-4)9(15-3)5-18-10/h9-12H,5-6
InchiKey: ZNZSWXTZXLFHNR-KXNHARMFSA-N
Formula: C12H20O7
SMILES: COC1COC(COC(C)=O)C(OC(C)=O)C1OC
Mol. weight [g/mol]: 276.28
CAS: 102803-54-3

Physical Properties

Property code	Value	Unit	Source
gf	-712.48	kJ/mol	Joback Method
hf	-1183.75	kJ/mol	Joback Method
hfus	37.81	kJ/mol	Joback Method
hvap	69.45	kJ/mol	Joback Method
log10ws	-0.17		Crippen Method
logp	-0.090		Crippen Method
mcvol	201.570	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
rinpol	1685.29		NIST Webbook
tb	703.87	K	Joback Method
tc	903.99	K	Joback Method
tf	435.01	K	Joback Method
vc	0.743	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.82	J/mol×K	703.87	Joback Method
cpg	678.02	J/mol×K	870.64	Joback Method
cpg	665.42	J/mol×K	837.28	Joback Method
cpg	651.67	J/mol×K	803.93	Joback Method
cpg	636.79	J/mol×K	770.58	Joback Method
cpg	620.83	J/mol×K	737.22	Joback Method
cpg	689.40	J/mol×K	903.99	Joback Method

dvisc	0.0001563	Pa×s	703.87	Joback Method
dvisc	0.0001902	Pa×s	659.06	Joback Method
dvisc	0.0002380	Pa×s	614.25	Joback Method
dvisc	0.0003087	Pa×s	569.44	Joback Method
dvisc	0.0004185	Pa×s	524.63	Joback Method
dvisc	0.0006006	Pa×s	479.82	Joback Method
dvisc	0.0009285	Pa×s	435.01	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=C102803543&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