1,5-Anhydro-3-o-acetyl-2,4,6-tri-o-methyl-d-glucito

Other names: 3-O-Acetyl-1,5-anhydro-2,4,6-tri-O-methyl-D-glucitol
Inchi: InChI=1S/C11H20O6/c1-7(12)17-11-8(14-3)6-16-9(5-13-2)10(11)15-4/h8-11H,5-6H2,1-4
InchiKey: UHHBRTSQTUOMIP-VPOLOUISSA-N
Formula: C11H20O6
SMILES: COC[C@H]1OC[C@H](OC)[C@H](OC(C)=O)[C@@H]1OC
Mol. weight [g/mol]: 248.28

Physical Properties

Property code	Value	Unit	Source
hfus	33.62	kJ/mol	Joback Method
logp	-0.007		Crippen Method
mcvol	185.910	ml/mol	McGowan Method
rinpol	1566.13		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.85	J/mol×K	627.12	Joback Method
cpg	543.85	J/mol×K	659.71	Joback Method
cpg	561.01	J/mol×K	692.29	Joback Method
cpg	577.30	J/mol×K	724.88	Joback Method
cpg	592.68	J/mol×K	757.46	Joback Method
cpg	607.10	J/mol×K	790.05	Joback Method
cpg	620.52	J/mol×K	822.64	Joback Method
dvisc	0.0010224	Pa×s	373.81	Joback Method
dvisc	0.0006464	Pa×s	416.03	Joback Method
dvisc	0.0004447	Pa×s	458.25	Joback Method
dvisc	0.0003259	Pa×s	500.47	Joback Method
dvisc	0.0002506	Pa×s	542.68	Joback Method
dvisc	0.0002002	Pa×s	584.90	Joback Method
dvisc	0.0001648	Pa×s	627.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97275519&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices