1,5-Anhydro-3,6-di-o-acetyl-2,4-di-o-methyl-d-gluc

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

Physical Properties

Property code	Value	Unit	Source
hfus	37.81	kJ/mol	Joback Method
logp	-0.090		Crippen Method
mcvol	201.570	ml/mol	McGowan Method
rinpol	1738.59		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.82	J/mol×K	703.87	Joback Method
cpg	620.83	J/mol×K	737.22	Joback Method
cpg	636.79	J/mol×K	770.58	Joback Method
cpg	651.67	J/mol×K	803.93	Joback Method
cpg	665.42	J/mol×K	837.28	Joback Method
cpg	678.02	J/mol×K	870.64	Joback Method
cpg	689.40	J/mol×K	903.99	Joback Method
dvisc	0.0009285	Pa×s	435.01	Joback Method
dvisc	0.0006006	Pa×s	479.82	Joback Method
dvisc	0.0004185	Pa×s	524.63	Joback Method
dvisc	0.0003087	Pa×s	569.44	Joback Method
dvisc	0.0002380	Pa×s	614.25	Joback Method
dvisc	0.0001902	Pa×s	659.06	Joback Method
dvisc	0.0001563	Pa×s	703.87	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97275531&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):	

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