1,5-Anhydro-4-O-acetyl-2,3,6-tri-O-methyl-D-mann

Other names: D-Mannitol, 1,5-anhydro-2,3,6-tri-O-methyl-, acetate
4-O-Acetyl-1,5-anhydro-2,3,6-tri-O-methyl-D-mannitol
Inchi: InChI=1S/C11H20O6/c1-7(12)17-11-9(5-13-2)16-6-8(14-3)10(11)15-4/h8-11H,5-6H2,1-4
InchiKey: BPVFAUHKDUHQHN-CHWFTXMASA-N
Formula: C11H20O6
SMILES: COCC1OCC(OC)C(OC)C1OC(C)=O
Mol. weight [g/mol]: 248.27
CAS: 102850-61-3

Physical Properties

Property code	Value	Unit	Source
gf	-591.98	kJ/mol	Joback Method
hf	-1050.53	kJ/mol	Joback Method
hfus	33.62	kJ/mol	Joback Method
hvap	60.48	kJ/mol	Joback Method
log10ws	0.02		Crippen Method
logp	-0.007		Crippen Method
mcvol	185.910	ml/mol	McGowan Method
pc	2100.34	kPa	Joback Method
rinpol	1600.00		NIST Webbook
tb	627.12	K	Joback Method
tc	822.64	K	Joback Method
tf	373.81	K	Joback Method
vc	0.680	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.85	J/mol×K	627.12	Joback Method
cpg	607.10	J/mol×K	790.05	Joback Method
cpg	592.68	J/mol×K	757.46	Joback Method
cpg	577.30	J/mol×K	724.88	Joback Method
cpg	561.01	J/mol×K	692.29	Joback Method
cpg	543.85	J/mol×K	659.71	Joback Method

cpg	620.52	J/mol×K	822.64	Joback Method
dvisc	0.0001648	Pa×s	627.12	Joback Method
dvisc	0.0002002	Pa×s	584.90	Joback Method
dvisc	0.0002506	Pa×s	542.68	Joback Method
dvisc	0.0003259	Pa×s	500.47	Joback Method
dvisc	0.0004447	Pa×s	458.25	Joback Method
dvisc	0.0006464	Pa×s	416.03	Joback Method
dvisc	0.0010224	Pa×s	373.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C102850613&Units=SI
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

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

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