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

Other names: D-Glucitol, 1,5-anhydro-3,4,6-tri-O-methyl-, acetate
2-O-Acetyl-1,5-anhydro-3,4,6-tri-O-methyl-D-glucitol
Inchi: InChI=1S/C11H20O6/c1-7(12)17-9-6-16-8(5-13-2)10(14-3)11(9)15-4/h8-11H,5-6H2,1-4H
InchiKey: GIVHIFDRSITQPC-YTWAJWBKSA-N
Formula: C11H20O6
SMILES: COCC1OCC(OC(C)=O)C(OC)C1OC
Mol. weight [g/mol]: 248.27
CAS: 102850-60-2

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	1537.86		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

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C102850602&Units=SI

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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