

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

Other names:	4-O-acetyl-1,5-Anhydro-2,3,6-tri-O-methyl-D-glucitol
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-ZRUFSTJUSA-N
Formula:	C11H20O6
SMILES:	COCC1OCC(OC)C(OC)C1OC(C)=O
Mol. weight [g/mol]:	248.27
CAS:	81847-57-6

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	1530.28		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/molxK	627.12	Joback Method
cpg	607.10	J/molxK	790.05	Joback Method
cpg	592.68	J/molxK	757.46	Joback Method
cpg	577.30	J/molxK	724.88	Joback Method
cpg	561.01	J/molxK	692.29	Joback Method
cpg	543.85	J/molxK	659.71	Joback Method
cpg	620.52	J/molxK	822.64	Joback Method

dvisc	0.0001648	Paxs	627.12	Joback Method
dvisc	0.0002002	Paxs	584.90	Joback Method
dvisc	0.0002506	Paxs	542.68	Joback Method
dvisc	0.0003259	Paxs	500.47	Joback Method
dvisc	0.0004447	Paxs	458.25	Joback Method
dvisc	0.0006464	Paxs	416.03	Joback Method
dvisc	0.0010224	Paxs	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=C81847576&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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