

1,5-Anhydro-d-glucitol, tetra-O-acetyl-

Other names:	2,6-Anhydro-L-gulitol peracetate 2,3,4,6-Tetra-O-acetyl-1,5-anhydro-D-glucitol D-Glucitol, 1,5-anhydro-, tetraacetate
Inchi:	InChI=1S/C14H20O9/c1-7(15)19-5-11-13(22-9(3)17)14(23-10(4)18)12(6-20-11)21-8(2)16
InchiKey:	ULWHEXUWXLOVPV-RQJABVFESA-N
Formula:	C14H20O9
SMILES:	CC(=O)OCC1OCC(OC(C)=O)C(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]:	332.30
CAS:	13137-69-4

Physical Properties

Property code	Value	Unit	Source
gf	-953.48	kJ/mol	Joback Method
hf	-1450.19	kJ/mol	Joback Method
hfus	46.19	kJ/mol	Joback Method
hvap	87.39	kJ/mol	Joback Method
log10ws	-0.56		Crippen Method
logp	-0.257		Crippen Method
mcvol	232.890	ml/mol	McGowan Method
pc	1921.98	kPa	Joback Method
rinpol	1894.83		NIST Webbook
tb	857.37	K	Joback Method
tc	1068.31	K	Joback Method
tf	557.41	K	Joback Method
vc	0.867	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.06	J/mol×K	857.37	Joback Method
cpg	802.73	J/mol×K	1033.15	Joback Method
cpg	795.81	J/mol×K	997.99	Joback Method
cpg	787.24	J/mol×K	962.84	Joback Method
cpg	777.05	J/mol×K	927.68	Joback Method

cpg	765.31	J/mol×K	892.53	Joback Method
cpg	807.95	J/mol×K	1068.31	Joback Method
dvisc	0.0001233	Pa×s	857.37	Joback Method
dvisc	0.0001499	Pa×s	807.38	Joback Method
dvisc	0.0001871	Pa×s	757.38	Joback Method
dvisc	0.0002409	Pa×s	707.39	Joback Method
dvisc	0.0003224	Pa×s	657.40	Joback Method
dvisc	0.0004526	Pa×s	607.40	Joback Method
dvisc	0.0006753	Pa×s	557.41	Joback Method

Sources

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=C13137694&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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