

1,5-Anhydroglucitol

Other names:	1,5-Anhydro-D-glucitol D-Glucitol, 1,5-anhydro- 1-Deoxy-D-glucopyranose
Inchi:	InChI=1S/C6H12O5/c7-1-4-6(10)5(9)3(8)2-11-4/h3-10H,1-2H2
InchiKey:	MPCAJMNYNNOGXPB-UHFFFAOYSA-N
Formula:	C6H12O5
SMILES:	OCC1OCC(O)C(O)C1O
Mol. weight [g/mol]:	164.16
CAS:	154-58-5

Physical Properties

Property code	Value	Unit	Source
gf	-632.44	kJ/mol	Joback Method
hf	-914.79	kJ/mol	Joback Method
hfus	30.67	kJ/mol	Joback Method
hvap	99.68	kJ/mol	Joback Method
log10ws	1.18		Crippen Method
logp	-2.540		Crippen Method
mcvol	113.890	ml/mol	McGowan Method
pc	5661.74	kPa	Joback Method
tb	737.89	K	Joback Method
tc	914.27	K	Joback Method
tf	421.89	K	Joback Method
vc	0.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.40	J/molxK	737.89	Joback Method
cpg	407.58	J/molxK	884.87	Joback Method
cpg	401.13	J/molxK	855.47	Joback Method
cpg	394.19	J/molxK	826.08	Joback Method
cpg	386.76	J/molxK	796.68	Joback Method
cpg	378.83	J/molxK	767.29	Joback Method

cpg	413.53	J/mol×K	914.27	Joback Method
dvisc	0.0000017	Paxs	737.89	Joback Method
dvisc	0.0000036	Paxs	685.22	Joback Method
dvisc	0.0000088	Paxs	632.56	Joback Method
dvisc	0.0000254	Paxs	579.89	Joback Method
dvisc	0.0000904	Paxs	527.22	Joback Method
dvisc	0.0004256	Paxs	474.56	Joback Method
dvisc	0.0029512	Paxs	421.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C154585&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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