D-cellobiose

Other names:	4-O-.beta.-D-glucopyranosyl-D-glucose D-(+)-cellobiose D-glucose, 4-O-.beta.-D-glucopyranosyl- cellobiose cellose
Inchi:	InChI=1S/C12H22O11/c13-1-3-5(15)6(16)9(19)12(22-3)23-10-4(2-14)21-11(20)8(18)7(10
InchiKey:	GUBGYTABKSRVRQ-BPUYHBCVSA-N
Formula:	C12H22O11
SMILES:	OCC1OC(OC2C(CO)OC(O)C(O)C2O)C(O)C(O)C1O
Mol. weight [g/mol]:	342.30
CAS:	528-50-7

Physical Properties

Property code	Value	Unit	Source
chs	-5401.50	kJ/mol	NIST Webbook
gf	-1334.42	kJ/mol	Joback Method
hf	-1959.15	kJ/mol	Joback Method
hfus	68.92	kJ/mol	Joback Method
hvap	185.55	kJ/mol	Joback Method
log10ws	1.89		Crippen Method
logp	-5.397		Crippen Method
mcvol	222.790	ml/mol	McGowan Method
pc	4311.22	kPa	Joback Method
tb	1289.46	K	Joback Method
tc	1783.82	K	Joback Method
tf	767.77	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	889.71	J/mol×K	1289.46	Joback Method
cpg	874.12	J/mol×K	1371.85	Joback Method
cpg	848.56	J/mol×K	1454.25	Joback Method

cpg	812.80	J/mol×K	1536.64	Joback Method
cpg	766.60	J/mol×K	1619.03	Joback Method
cpg	709.75	J/mol×K	1701.43	Joback Method
cpg	641.99	J/mol×K	1783.82	Joback Method
cps	534.80	J/mol×K	358.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	431.00	J/mol×K	293.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	436.10	J/mol×K	298.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	445.00	J/mol×K	303.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	443.10	J/mol×K	308.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	446.90	J/mol×K	313.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	448.70	J/mol×K	318.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	463.20	J/mol×K	323.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides

cps	407.80	J/mol×K	288.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	473.10	J/mol×K	333.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	481.10	J/mol×K	338.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	490.70	J/mol×K	343.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	503.20	J/mol×K	348.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	515.80	J/mol×K	353.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	463.50	J/mol×K	328.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
dvisc	2.0238363e-08	Pa×s	767.77	Joback Method
dvisc	3.1497617e-09	Pa×s	854.72	Joback Method
dvisc	6.9115221e-10	Pa×s	941.67	Joback Method
dvisc	1.9598804e-10	Pa×s	1028.62	Joback Method
dvisc	6.7640490e-11	Pa×s	1115.56	Joback Method
dvisc	2.7226863e-11	Pa×s	1202.51	Joback Method
dvisc	1.2390430e-11	Pa×s	1289.46	Joback Method
hsubt	302.00 ± 44.00	kJ/mol	481.00	NIST Webbook

Sources

Studies on the Interactions of Saccharides and Methyl Glycosides with Lithium Chloride in Aqueous Solutions at 298.15 K:	https://www.doi.org/10.1021/je5001523
Apparent molar volumes and apparent molar heat capacities of aqueous solutions of D(+) cellobiose, D(+) maltose, and sucrose at temperatures from 278.15 K to 318.15 K and at the pressure 0.35 MPa:	https://www.doi.org/10.1016/j.jct.2004.12.004
Volumetric Properties of Disaccharides in Aqueous Solutions of Urea at Temperatures from 278.15 K to 318.15 K and at the Pressure 0.35 MPa:	https://www.doi.org/10.1021/je501169y
Volumetric and Viscometric Studies on Saccharides in Aqueous Sodium Tetraborate (Borax) Solutions at Different Temperatures:	https://www.doi.org/10.1021/je400264a
Densities and Viscosities of Some Saccharides in Aqueous Potassium Chloride Solutions over Temperature Range (288.15 to 318.15) K:	https://www.doi.org/10.1016/j.jct.2008.11.009
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Modulation in physico-chemical characteristics of some polyhydroxy solutes in presence of L-glycine: Volumetric and NMR spectroscopic approach:	https://www.doi.org/10.1016/j.fluid.2015.05.043
Viscometric studies on saccharides in aqueous magnesium chloride solutions at (288.15 to 318.15) K:	https://www.doi.org/10.1016/j.jct.2012.02.016
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Effect of sodium acetate on the volumetric behaviour of some mono-, di-, and tri-saccharides in aqueous solutions over the temperature range (288.15 to 318.15) K:	https://www.doi.org/10.1016/j.jct.2009.07.015
Solid-Liquid Equilibrium of Cellobiose, Sucrose, and Maltose Monohydrate in Mixtures of Methanol and Water: Experimental and Quantum Chemical Insights:	https://www.doi.org/10.1021/acs.jced.5b00914
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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Thermodynamic Study of Some Amino Acids, 2-Aminopropanoic Acid, 2-Amino-3-methylbutanoic Acid, 2-Aminohexanoic Acid, and 2-Amino-5-methylhexanoic Acid in Aqueous Solutions of Biological Buffer (Bis-tris) at Different Temperatures:	https://www.doi.org/10.1021/je100857s
Viscosities of Some Saccharides in Aqueous Solutions of Glycylglycine at Different Temperatures:	https://www.doi.org/10.1021/acs.jced.5b00845
Rotational-echo double-resonance relaxation studies of some polyhydroxy solutes in the presence of L-glycine:	https://www.doi.org/10.1016/j.jct.2016.04.006
Aqueous Saccharide Solutions at Different Temperatures. Volumetric and Ultrasonic Study:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C528507&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase 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
hsubt:	Enthalpy of sublimation at a given temperature
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