Xylitol

Other names:	klinit
	kylit
	xylite
	xyliton
Inchi:	InChI=1S/C5H12O5/c6-1-3(8)5(10)4(9)2-7/h3-10H,1-2H2/t3-,4+,5+
InchiKey:	HEBKCHPVOIAQTA-SCDXWVJYSA-N
Formula:	C5H12O5
SMILES:	OCC(O)C(O)C(O)CO
Mol. weight [g/mol]:	152.15
CAS:	87-99-0

Physical Properties

Property code	Value	Unit	Source
chl	-2564.00 ± 0.63	kJ/mol	NIST Webbook
gf	-700.20	kJ/mol	Joback Method
hf	-923.52	kJ/mol	Joback Method
hfl	-1118.60 ± 0.63	kJ/mol	NIST Webbook
hfus	33.68	kJ/mol	Thermodynamic investigation of several natural polyols (I): Heat capacities and thermodynamic properties of xylitol
hsub	161.00	kJ/mol	NIST Webbook
hvap	108.95	kJ/mol	Joback Method
log10ws	1.43		Crippen Method
logp	-2.946		Crippen Method
mcvol	110.660	ml/mol	McGowan Method
pc	6785.20	kPa	Joback Method
tb	773.38	K	Joback Method
tc	947.56	K	Joback Method
tf	367.20	K	Solubility data and modeling for sugar alcohols in ionic liquids
tf	366.10	K	Heat capacities of some sugar alcohols as phase change materials for thermal energy storage applications

tf	366.20	K	Experimental and in silico characterization of xylitol as seasonal heat storage material
tf	367.20	K	Solid-liquid phase equilibria in binary mixtures of functionalized ionic liquids with sugar alcohols: New experimental data and modelling
tf	367.65	K	Solubility of Xylitol in Ethanol, Acetone, N,N-Dimethylformamide, 1-Butanol, 1-Pentanol, Toluene, 2-Propanol, and Water
tf	367.65	K	Measurement and Correlation of Solubility of Xylitol in Binary Ethanol + Acetone Solvent Mixtures with the Combined Nearly Ideal Binary Solvent/ Redlich-Kister Equation
tf	365.70 ± 0.20	K	NIST Webbook
vc	0.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.45	J/mol×K	918.53	Joback Method
cpg	364.86	J/mol×K	947.56	Joback Method
cpg	334.42	J/mol×K	773.38	Joback Method
cpg	340.20	J/mol×K	802.41	Joback Method
cpg	345.68	J/mol×K	831.44	Joback Method
cpg	350.87	J/mol×K	860.47	Joback Method
cpg	355.79	J/mol×K	889.50	Joback Method
dvisc	0.0000003	Pa×s	712.02	Joback Method
dvisc	0.0000001	Pa×s	773.38	Joback Method
dvisc	0.0076529	Pa×s	405.21	Joback Method
dvisc	0.0003514	Pa×s	466.57	Joback Method
dvisc	0.0000330	Pa×s	527.93	Joback Method
dvisc	0.0000051	Pa×s	589.30	Joback Method
dvisc	0.0000011	Pa×s	650.66	Joback Method
hfust	37.40	kJ/mol	365.70	NIST Webbook
hfust	37.70	kJ/mol	368.00	NIST Webbook
hfust	37.40	kJ/mol	365.70	NIST Webbook
hfust	33.26	kJ/mol	369.00	NIST Webbook

hvapt	111.10 ± 0.80	kJ/mol	433.00	NIST Webbook
sfust	102.30	J/mol×K	365.70	NIST Webbook

Sources

Densities and Viscosities of Sugar Alcohol Aqueous Solutions:	https://www.doi.org/10.1021/je9010486
Investigations to explore interactions in (polyhydroxy solute + L-ascorbic acid + H2O) solutions at different temperatures: Calorimetric and viscometric approach:	https://www.doi.org/10.1016/j.jct.2016.07.020
Solubility Behavior and Data Modeling of l-Proline in Different Neat and Binary Solvent Systems:	https://www.doi.org/10.1021/acs.jced.9b00802
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Densities and Viscosities of Sugar Alcohols in Vitamin B6 Aqueous Solutions at (298.15 to 323.15) K:	https://www.doi.org/10.1021/acs.jced.5b00114
Densities and Viscosities of Erythritol, Xylitol, and Mannitol in l-ascorbic Acid Aqueous Solutions at T = (293.15 to 323.15) K:	https://www.doi.org/10.1021/je400395u
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Densities and Viscosities of Polyhydroxy Solutes in Aqueous Tetraethylammonium Bromide Solutions at Different Temperatures:	https://www.doi.org/10.1021/acs.jced.5b00940
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Solid-liquid phase equilibria in binary mixtures of functionalized ionic liquids with sugar alcohols: New experimental data and modelling:	https://www.doi.org/10.1016/j.fluid.2015.06.002
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Solubility of xylitol and sorbitol in ionic liquids - Experimental data and modeling:	https://www.doi.org/10.1016/j.jct.2012.05.020
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87990&Units=SI
Enthalpies of Dilution, Volumetric Properties, and Refractive Indices of N,N'-Hexamethylenebisacetamide in Aqueous Xylitol or d-Mannitol Solutions at T = 298.15 K:	https://www.doi.org/10.1021/je300633e
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Density of Mixtures Containing Sugars and Ionic Liquids: Experimental Data and PC-SAFT Modeling:	https://www.doi.org/10.1021/je500079y
Partitioning of diuron in a novel aqueous two-phase system based on polyols and tetrahydrofuran:	https://www.doi.org/10.1016/j.fluid.2016.08.012
Heat capacities of some sugar alcohols as phase change materials for thermal energy storage applications:	https://www.doi.org/10.1016/j.jct.2017.08.004
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Enthalpy of dilution and volumetric properties of N-glycylglycine in aqueous xylitol solutions at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2011.02.005
Properties of Sugar, Polyol, and Polysaccharide Water-Ethanol Solutions:	https://www.doi.org/10.1021/je700190m
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Solubility of Xylitol in Ethanol, Acetone, N,N-Dimethylformamide, 1-Butanol, 1-Pentanol, Toluene, 2-Propanol, and Water:	https://www.doi.org/10.1021/je060348v
Apparent molar volumes and apparent molar heat capacities of aqueous adonitol, dulcitol, glycerol, meso-erythritol, myo-inositol, D-sorbitol and xylitol at temperatures from (278.15 to 368.15) K and at the pressure 0.35 MPa:	https://www.doi.org/10.1016/j.jct.2006.08.009
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Osmotic properties of carbohydrate aqueous solutions:	https://www.doi.org/10.1016/j.fluid.2016.02.030
Solubility data and modeling for sugar alcohols in ionic liquids:	https://www.doi.org/10.1016/j.jct.2014.04.021
Experimental and in silico characterization of xylitol as seasonal heat storage material:	https://www.doi.org/10.1016/j.fluid.2016.12.020

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume