L-Sorbose

Other names:	Esorben
	Hex-2-ulose, L-xylo-
	L-(-)-sorbose
	L-1,3,4,5,6-pentahydroxyhexan-2-one
	L-Sorbinose
	NSC 97195
	Sorbin
	Sorbinose
	Sorbose
	Sorbose, L-
	l-Xylo-2-hexulose
Inchi:	InChI=1S/C6H12O6/c7-1-3(9)5(11)6(12)4(10)2-8/h3,5-9,11-12H,1-2H2/t3-,5+,6+/m1/s1
InchiKey:	BJHIKXHVCXFQLS-PYWDMBMJSA-N
Formula:	C6H12O6
SMILES:	O=C(CO)C(O)C(O)C(O)CO
Mol. weight [g/mol]:	180.16
CAS:	87-79-6

Physical Properties

Property code	Value	Unit	Source
chs	-2799.10 ± 1.00	kJ/mol	NIST Webbook
chs	-2804.50 ± 0.40	kJ/mol	NIST Webbook
gf	-820.70	kJ/mol	Joback Method
hf	-1056.74	kJ/mol	Joback Method
hfs	-1276.90 ± 1.00	kJ/mol	NIST Webbook
hfs	-1271.50 ± 0.50	kJ/mol	NIST Webbook
hfus	22.77	kJ/mol	Joback Method
hvap	117.93	kJ/mol	Joback Method
log10ws	1.73		Crippen Method
logp	-3.377		Crippen Method
mcvol	126.320	ml/mol	McGowan Method
pc	6430.83	kPa	Joback Method
ss	220.90	J/mol×K	NIST Webbook
tb	850.13	K	Joback Method
tc	1041.01	K	Joback Method
tf	466.41	K	Joback Method
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.42	J/mol×K	850.13	Joback Method
cpg	418.30	J/mol×K	1041.01	Joback Method
cpg	414.12	J/mol×K	1009.20	Joback Method
cpg	409.65	J/mol×K	977.39	Joback Method
cpg	404.87	J/mol×K	945.57	Joback Method
cpg	399.74	J/mol×K	913.76	Joback Method
cpg	394.27	J/mol×K	881.94	Joback Method
cps	228.61	J/mol×K	295.90	NIST Webbook
dvisc	4.5130364e-08	Pa×s	850.13	Joback Method
dvisc	0.0000001	Pa×s	786.18	Joback Method
dvisc	0.0000004	Pa×s	722.22	Joback Method
dvisc	0.0000013	Pa×s	658.27	Joback Method
dvisc	0.0000066	Pa×s	594.32	Joback Method
dvisc	0.0000482	Pa×s	530.36	Joback Method
dvisc	0.0006126	Pa×s	466.41	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Influence of NH4Br on Solvation Behavior of Polyhydroxy Solutes in Aqueous Solutions at Different Temperatures and Atmospheric Pressure:	https://www.doi.org/10.1021/je500886a
McGowanMethod:	http://link.springer.com/article/10.1007/BF02311772
Densities and Viscosities of Polyhydroxy Solutes in Aqueous Tetraethylammonium Bromide Solutions at Different Temperatures:	https://www.doi.org/10.1021/acs.jced.5b00940
Volumetric and Viscometric Studies on Saccharides in Disodium Tetraborate (Borax) Interactions in Aqueous Solutions:	https://www.doi.org/10.1021/je400264a
Modulation in physico-chemical characteristics of some polyhydroxy solutes in presence of L-glycine: Volumetric, viscometric and 1H NMR spectroscopic approach:	https://www.doi.org/10.1016/j.fluid.2015.05.043
Volumetric, viscometric and 1H NMR spectroscopic studies in polyhydroxy solutes in (TAB + H2O) ternary solutions:	https://www.doi.org/10.1016/j.jct.2017.04.001
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87796&Units=SI
Effect of sodium acetate on the volumetric behaviour of some mono-, di-, and tri-saccharides in aqueous solutions over temperature range (288.15 to 318.15) K:	https://www.doi.org/10.1016/j.jct.2009.07.015
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hfs:	Solid phase 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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume