Sucrose

Other names:

(+)-Sucrose (2R,3R,4S,5S,6R)-2-(((2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)tetrahydrofura («alpha»-D-Glucosido)-«beta»-D-fructofuranoside («alpha»-D-Glucosido)-«beta»-D-fructofuranoside .alpha.-trehalose .beta.-D-fructofuranosyl .alpha.-D-glucopyranoside 4-O-.beta.-D-galactopyranosyl-D-glucose Amerfond Beet sugar Cane sugar Confectioner's sugar D-(+)-Saccharose D-(+)-Sucrose D-(+)-lactose **D-Sucrose** D-trehalose Fructofuranoside, «alpha»-D-glucopyranosyl, «beta»-D Fructofuranoside, «alpha»-D-glucopyranosyl, «beta»-D Glucopyranoside, «beta»-D-fructofuranosyl, «alpha»-D Glucopyranoside, «beta»-D-fructofuranosyl, «alpha»-D Granulated sugar Microse NCI-C56597 NSC 406942 Rock candy Saccharose Saccharum Sugar Table sugar White sugar alpha, alpha-trehalose lactose «alpha»-D-Glucopyranoside, «beta»-D-fructofuranosyl «alpha»-D-Glucopyranosyl «beta»-D-fructofuranoside «beta»-D-Fructofuranoside, «alpha»-D-glucopyranosyl «beta»-D-Fructofuranosyl «alpha»-D-glucopyranoside «alpha»-D-Glucopyranoside, «beta»-D-fructofuranosyl «alpha»-D-Glucopyranosyl «beta»-D-fructofuranoside «beta»-D-Fructofuranoside, «alpha»-D-glucopyranosyl «beta»-D-Fructofuranosyl «alpha»-D-glucopyranoside

Inchi:	InChI=1S/C12H22O11/c13-1-4-6(16)8(18)9(19)11(21-4)23-12(3-15)10(20)7(17)5(2-14)22
InchiKey:	CZMRCDWAGMRECN-SFOFJGFUSA-N
Formula:	C12H22O11
SMILES:	OCC1OC(OC2(CO)OC(CO)C(O)C2O)C(O)C(O)C1O
Mol. weight [g/mol]:	342.30
CAS:	57-50-1

Physical Properties

Property code	Value	Unit	Source
chs	-5664.38 ± 0.69	kJ/mol	NIST Webbook
chs	-5637.40 ± 1.70	kJ/mol	NIST Webbook
chs	-5644.17	kJ/mol	NIST Webbook
chs	-5643.40 ± 1.80	kJ/mol	NIST Webbook
gf	-1320.10	kJ/mol	Joback Method
hf	-1917.41	kJ/mol	Joback Method
hfs	-2221.20	kJ/mol	NIST Webbook
hfus	63.65	kJ/mol	Joback Method
hvap	184.54	kJ/mol	Joback Method
log10ws	0.79		Estimated Solubility Method
log10ws	0.79		Aqueous Solubility Prediction Method
logp	-5.396		Crippen Method
mcvol	222.790	ml/mol	McGowan Method
рс	4627.70	kPa	Joback Method
SS	392.40	J/mol×K	NIST Webbook
SS	360.20	J/mol×K	NIST Webbook
tb	1290.10	К	Joback Method
tc	1782.75	К	Joback Method
tf	462.00 ± 3.00	К	NIST Webbook
tf	424.40	К	Heat capacity and transition behavior of sucrose by standard, fast scanning and temperature-modulated calorimetry
tf	464.05	К	Artificial neural networks as a supporting tool for compatibility study based on thermogravimetric data
tf	461.00 ± 6.00	К	NIST Webbook
tf	458.65	К	Aqueous Solubility Prediction Method
VC	0.784	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1178.26	J/mol×K	1782.75	Joback Method
cpg	970.71	J/mol×K	1290.10	Joback Method
срд	998.85	J/mol×K	1372.21	Joback Method
cpg	1028.30	J/mol×K	1454.32	Joback Method
cpg	1060.01	J/mol×K	1536.42	Joback Method
cpg	1094.94	J/mol×K	1618.53	Joback Method
cpg	1134.04	J/mol×K	1700.64	Joback Method
cps	422.50	J/mol×K	297.00	NIST Webbook
cps	408.50	J/mol×K	288.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	416.60	J/mol×K	293.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	424.30	J/mol×K	298.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	429.40	J/mol×K	303.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	437.50	J/mol×K	308.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides

cps	445.50	J/mol×K	313.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides	
cps	451.00	J/mol×K	318.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides	
cps	466.20	J/mol×K	323.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides	
cps	472.60	J/mol×K	328.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides	
cps	482.50	J/mol×K	333.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides	
cps	490.30	J/mol×K	338.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides	
cps	498.80	J/mol×K	343.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides	
cps	506.70	J/mol×K	348.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides	
cps	513.90	J/mol×K	353.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides	

cps	522.00	J/mol×K	358.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides	
cps	424.30	J/mol×K	298.15	NIST Webbook	
cps	430.00	J/mol×K	300.00	NIST Webbook	
cps	425.50	J/mol×K	298.15	NIST Webbook	
hfust	46.20	kJ/mol	459.00	NIST Webbook	

Sources

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Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
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
hfust:	Enthalpy of fusion 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
SS:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
VC:	Critical Volume

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