Erythritol

Other names:	(R*,S*)-1,2,3,4-butanetetrol 1,2,3,4-Butanetetrol, (2R,3S)-rel- 1,2,3,4-Butanetetrol, (R*,S*)- 1,2,3,4-Tetrahydroxybutane, (R*,S*)- 2(R),3(S)-1,2,3,4-Butanetetrol Antierythrite C*Eridex Erythrit Erythrite Erythritol, meso- Erythroglucin Erythrol L-Erythritol Lichen sugar NIK 242 NSC 8099 Paycite Phycitol TETRAHYDOXYBUTANE meso-1,2,3,4-butanetetrol meso-Erythritol
Inchi:	InChI=1S/C4H10O4/c5-1-3(7)4(8)2-6/h3-8H,1-2H2/t3-,4+
InchiKey:	UNXHWFMMPAWVPI-ZXZARUISSA-N
Formula:	C4H10O4
SMILES:	OCC(O)C(O)CO
Mol. weight [g/mol]:	122.12
CAS:	149-32-6

Physical Properties

Property code	Value	Unit	Source
chl	-2092.80 ± 1.30	kJ/mol	NIST Webbook
chs	-2118.00	kJ/mol	NIST Webbook
gf	-569.36	kJ/mol	Joback Method
hf	-745.37	kJ/mol	Joback Method
hfl	-910.48 ± 0.54	kJ/mol	NIST Webbook

hfus	39.93	kJ/mol	Measurement of enthalpy curves of phase change materials via DSC and T-History: When are both methods needed to estimate the behaviour of the bulk material in applications?
hsub	140.00	kJ/mol	NIST Webbook
hsub	157.00	kJ/mol	NIST Webbook
hsub	135.00	kJ/mol	NIST Webbook
hvap	93.30	kJ/mol	NIST Webbook
log10ws	0.70		Aqueous Solubility Prediction Method
log10ws	0.70		Estimated Solubility Method
logp	-2.307		Crippen Method
mcvol	90.700	ml/mol	McGowan Method
pc	6740.71	kPa	Joback Method
ss	177.80	J/mol×K	NIST Webbook
ss	166.50	J/mol×K	NIST Webbook
tb	603.70	K	NIST Webbook
tc	819.90	K	Joback Method
tf	391.60 ± 0.20	K	NIST Webbook
tf	390.50	K	Solid-liquid phase equilibria in binary mixtures of functionalized ionic liquids with sugar alcohols: New experimental data and modelling
tf	392.05	K	KDB
tf	394.90	K	Aqueous Solubility Prediction Method
tf	390.90 ± 0.20	K	NIST Webbook
tf	394.82	K	Heat capacities of some sugar alcohols as phase change materials for thermal energy storage applications
vc	0.324	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.00	J/mol×K	766.19	Joback Method
cpg	273.46	J/mol×K	793.04	Joback Method
cpg	248.93	J/mol×K	658.76	Joback Method

cpg	254.30	J/mol×K	685.62	Joback Method
cpg	259.43	J/mol×K	712.47	Joback Method
cpg	264.33	J/mol×K	739.33	Joback Method
cpg	277.70	J/mol×K	819.90	Joback Method
cps	170.70	J/mol×K	303.00	NIST Webbook
cps	161.90	J/mol×K	291.70	NIST Webbook
dvisc	0.0000058	Pa×s	606.99	Joback Method
dvisc	0.0000022	Pa×s	658.76	Joback Method
dvisc	0.0672433	Pa×s	348.12	Joback Method
dvisc	0.0039218	Pa×s	399.89	Joback Method
dvisc	0.0004388	Pa×s	451.67	Joback Method
dvisc	0.0000770	Pa×s	503.44	Joback Method
dvisc	0.0000187	Pa×s	555.21	Joback Method
hfust	40.30	kJ/mol	392.20	NIST Webbook
hfust	42.36	kJ/mol	396.00	NIST Webbook
hfust	39.40	kJ/mol	390.90	NIST Webbook
hfust	42.36	kJ/mol	381.60	NIST Webbook
hfust	38.90	kJ/mol	391.20	NIST Webbook
hvapt	93.30	kJ/mol	397.50	NIST Webbook
hvapt	113.60 ± 1.10	kJ/mol	412.50	NIST Webbook
hvapt	97.00 ± 1.00	kJ/mol	398.00	NIST Webbook
sfust	111.00	J/mol×K	381.60	NIST Webbook
sfust	100.80	J/mol×K	390.90	NIST Webbook

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Enthalpies of dilution of aqueous solutions of n-butanol, butanediols, 1,2,4-butanetriol, and 1,2,3,4-butanetetrol at 298.15K: https://www.doi.org/10.1016/j.tca.2005.06.014

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

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

Partitioning of durion in a novel aqueous two-phase system based on polyols and tetrahydrofuran: https://www.doi.org/10.1016/j.fluid.2016.08.012

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

Solubility of erythritol in methanol, ethanol and methanol + ethanol: Experimental measurement and thermodynamic modeling: https://www.doi.org/10.1016/j.fluid.2013.09.027

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C149326&Units=SI

Apparent molar volumes and apparent molar heat capacities of aqueous acetitol, dulcitol, glycerol, meso-erythritol, myo-inositol, D-sorbitol, and xylitol at temperatures from 278.15 K to 328.15 K and at pressure 0.35 MPa: https://www.doi.org/10.1016/j.jct.2006.08.009

Densities and Viscosities of Sugar Alcohol Aqueous Solutions: https://www.doi.org/10.1021/je9010486

Densities and Viscosities of Sugar Alcohols in Vitamin B6 Aqueous Solutions from (278.15 to 328.15) K and at Ambient Pressure: https://www.doi.org/10.1021/acs.jced.5b00114

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Isopiestic determination of osmotic and activity coefficients of aqueous solutions of aliphatic polyols at 298.15K: https://www.doi.org/10.1016/j.fluid.2005.12.016

Measurement of enthalpy curves of phase change materials via DSC and T-History: When are both methods needed to estimate the behaviour of the bulk material in applications?:	https://www.doi.org/10.1016/j.tca.2014.09.022
Solubility of Erythritol in Different Solvents:	https://www.doi.org/10.1021/je0501033
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=920
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
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
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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume