Pentaerythritol

Other names:	1,1,1-Tris(hydroxymethyl)ethanol 1,3-Propanediol, 2,2-bis(hydroxymethyl)- 2,2-Bis(hydroxymethyl)-1,3-propanediol Auxenutril Auxinutril Charmor PM 15 Hercules Mono-PE Hercules P6 Maxinutril Metab-Auxil Methane tetramethylol Methane, tetrakis(hydroxymethyl)-, Monopentaerythritol Monopentek NSC 8100 PE 200 PETP Penetek Pentaertyhritol Pentaerythrite Pentek THME Tetrahydroxymethylmethane Tetrakis(hydroxymethyl)methane Tetramethylolmethane tetramethylol methane
Inchi:	InChI=1S/C5H12O4/c6-1-5(2-7,3-8)4-9/h6-9H,1-4H2
InchiKey:	WXZMFSXDPGVJKK-UHFFFAOYSA-N
Formula:	C5H12O4
SMILES:	OCC(CO)(CO)CO
Mol. weight [g/mol]:	136.15
CAS:	115-77-5

Physical Properties

Property code	Value	Unit	Source
chs	-2762.00 ± 2.80	kJ/mol	NIST Webbook

gf	-553.22	kJ/mol	Joback Method
hf	-764.20	kJ/mol	Joback Method
hfs	-920.50 ± 2.80	kJ/mol	NIST Webbook
hfus	17.64	kJ/mol	Joback Method
hsub	163.00	kJ/mol	NIST Webbook
hvap	92.14	kJ/mol	Joback Method
log10ws	-0.44		Aqueous Solubility Prediction Method
logp	-2.058		Crippen Method
mcvol	104.790	ml/mol	McGowan Method
pc	5818.28	kPa	Joback Method
ss	198.07	J/mol×K	NIST Webbook
tb	679.29	K	Joback Method
tc	842.76	K	Joback Method
tf	538.70 ± 0.10	K	NIST Webbook
tf	529.00 ± 2.00	K	NIST Webbook
tf	531.00 ± 3.00	K	NIST Webbook
tf	531.20 ± 1.20	K	NIST Webbook
tf	532.77	K	Aqueous Solubility Prediction Method
tt	454.55	K	Experimental study on the thermal storage performance and non-isothermal crystallization kinetics of pentaerythritol blended with low melting metal
vc	0.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.17	J/mol×K	679.29	Joback Method
cpg	304.15	J/mol×K	706.53	Joback Method
cpg	309.83	J/mol×K	733.78	Joback Method
cpg	315.23	J/mol×K	761.02	Joback Method
cpg	320.37	J/mol×K	788.27	Joback Method
cpg	325.26	J/mol×K	815.51	Joback Method
cpg	329.92	J/mol×K	842.76	Joback Method
cps	188.40	J/mol×K	298.98	NIST Webbook
cps	190.41	J/mol×K	298.15	NIST Webbook
cps	254.40	J/mol×K	373.20	NIST Webbook
dvisc	0.0000016	Pa×s	679.29	Joback Method
dvisc	0.0008769	Pa×s	439.72	Joback Method

dvisc	0.0001501	Pa×s	487.64	Joback Method
dvisc	0.0078907	Pa×s	391.81	Joback Method
dvisc	0.0000105	Pa×s	583.46	Joback Method
dvisc	0.0000038	Pa×s	631.38	Joback Method
dvisc	0.0000352	Pa×s	535.55	Joback Method
hfust	7.11	kJ/mol	538.70	NIST Webbook
hfust	5.30	kJ/mol	532.30	NIST Webbook
hfust	4.60	kJ/mol	513.20	NIST Webbook
hfust	43.93	kJ/mol	460.40	NIST Webbook
hfust	7.11	kJ/mol	538.70	NIST Webbook
hsubt	131.30 ± 6.60	kJ/mol	403.00	NIST Webbook
hsubt	161.00 ± 1.00	kJ/mol	436.50	NIST Webbook
hsubt	143.90 ± 0.80	kJ/mol	393.50	NIST Webbook
sfust	95.40	J/mol×K	460.40	NIST Webbook
sfust	13.20	J/mol×K	538.70	NIST Webbook

Sources

Densimetric and ultrasonic characterization of pentaerythritol in water and in aqueous NaCl and MgCl2 solutions at different temperatures:	https://www.doi.org/10.1016/j.jct.2012.05.033
Experimental study on the thermal storage performance and thermal reliability of erythritol and erythritol blended with low melting metal:	https://www.doi.org/10.1016/j.tca.2018.02.007
Partial Molar Isentropic Compressions and Partial Molar Volumes of Selected Alkanols, Diols, and Cyclic Alcohols at Infinite Dilution in Water at Temperatures from T = (278 to 318) K and Atmospheric Pressure:	https://www.doi.org/10.1021/je300175w
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C115775&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfust:	Enthalpy of fusion at a given temperature

hsub:	Enthalpy of sublimation 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
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
tt:	Triple Point Temperature
vc:	Critical Volume