1,3-Propanediol, 2-ethyl-2-(hydroxymethyl)-

Other names: 1,1,1-Tri(hydroxymethyl)propane
1,1,1-Trimethylolpropane
1,1,1-Tris(Hydroxymethyl)propane
1,1,1-trihydroxymethylpropane
2,2-Bis(hydroxymethyl)-1-butanol
2,2-dihydroxymethyl-1-butanol
2-Ethyl-2-(hydroxymethyl)-1,3-propanediol
2-Ethyl-2-(hydroxymethyl)propanediol
Butanol, 2,2-bis(hydroxymethyl)-
Ethriol
Ethyltrimethylolmethane
Etriol
Ettriol
Hexaglycerine
Hexaglycerol
Methanol, (propanetriyl)tris-
NSC 3576
Propane, 1,1,1-tris(hydroxymethyl)-
TMP
TMP (Alcohol)
Tri(hydroxymethyl)propane
Trimethylolpropane
Tris(hydroxymethyl)propane
propylidynetrimethanol

Inchi: InChI=1S/C6H14O3/c1-2-6(3-7,4-8)5-9/h7-9H,2-5H2,1H3

InchiKey: ZJCCRDAZUWHFQH-UHFFFAOYSA-N

Formula: C6H14O3

SMILES: CCC(CO)(CO)CO

Mol. weight [g/mol]: 134.17

CAS: 77-99-6

Physical Properties

Property code	Value	Unit	Source
chs	-3611.00	kJ/mol	NIST Webbook
gf	-407.98	kJ/mol	Joback Method
hf	-632.61	kJ/mol	Joback Method

hfs	-746.40	kJ/mol	NIST Webbook
hfs	-751.00	kJ/mol	NIST Webbook
hfus	16.15	kJ/mol	Joback Method
hvap	77.69	kJ/mol	Joback Method
log10ws	0.12		Crippen Method
logp	-0.640		Crippen Method
mcvol	113.010	ml/mol	McGowan Method
pc	4450.38	kPa	Joback Method
tb	609.99	K	Joback Method
tc	772.16	K	Joback Method
tf	342.26	K	Joback Method
tt	333.40 ± 0.05	K	NIST Webbook
vc	0.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.94	J/mol×K	772.16	Joback Method
cpg	304.02	J/mol×K	609.99	Joback Method
cpg	325.99	J/mol×K	691.08	Joback Method
cpg	332.62	J/mol×K	718.11	Joback Method
cpg	338.93	J/mol×K	745.13	Joback Method
cpg	319.03	J/mol×K	664.05	Joback Method
cpg	311.71	J/mol×K	637.02	Joback Method
cps	213.79	J/mol×K	301.29	NIST Webbook
dvisc	0.0000112	Pa×s	609.99	Joback Method
dvisc	0.0000656	Pa×s	520.75	Joback Method
dvisc	0.0002028	Pa×s	476.12	Joback Method
dvisc	0.0007925	Pa×s	431.50	Joback Method
dvisc	0.0042401	Pa×s	386.88	Joback Method
dvisc	0.0000253	Pa×s	565.37	Joback Method
dvisc	0.0351304	Pa×s	342.26	Joback Method
hfust	21.45	kJ/mol	312.00	NIST Webbook
hfust	0.90	kJ/mol	332.70	NIST Webbook
hfust	21.45	kJ/mol	333.40	NIST Webbook
hvapt	81.40	kJ/mol	501.50	NIST Webbook
sfust	64.30	J/mol×K	333.40	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	433.20	K	0.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.10282e+01
Coeff. B	-9.34767e+03
Coeff. C	-5.15000e-01
Temperature range (K), min.	451.21
Temperature range (K), max.	595.27

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Liquid-Liquid Equilibria for the Ternary and Quaternary Systems of Water + Trimethylolpropane + (2-Ethylhexan-1-ol/Octan-1-ol) + Formaldehyde at 298.15 K:	https://www.doi.org/10.1021/acs.jced.9b00519
Partial Molar Isentropic Compressions and Partial Molar Volumes of Selected 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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77996&Units=SI

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
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
pvap:	Vapor pressure
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume