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

Other names:	1,1,1-trimethanolethane 1,1,1-trimethylolethane 1,1,1-tris(hydroxymethyl)ethane 1,1,1-tris(methylol)ethane 2,2-bis(hydroxymethyl)-1-propanol 2,2-di(hydroxymethyl)propanol 2-(hydroxymethyl)-2-methyl-1,3-propanediol Methriol Metriol NSC 65581 TME Trimet Tris(hydroxymethyl)ethane ethane, 1,1,1-tris(hydroxymethyl)- ethylidynetrimethanol methyltrimethanolmethane pentaglycerine trimethylolethane
Inchi:	InChI=1S/C5H12O3/c1-5(2-6,3-7)4-8/h6-8H,2-4H2,1H3
InchiKey:	QXJQHYBHAIHNGG-UHFFFAOYSA-N
Formula:	C5H12O3
SMILES:	CC(CO)(CO)CO
Mol. weight [g/mol]:	120.15
CAS:	77-85-0

Physical Properties

Property code	Value	Unit	Source
chs	-2938.00 ± 2.90	kJ/mol	NIST Webbook
chs	-2941.80	kJ/mol	NIST Webbook
gf	-416.40	kJ/mol	Joback Method
hf	-611.97	kJ/mol	Joback Method
hfs	-744.30 ± 3.00	kJ/mol	NIST Webbook
hfs	-740.78	kJ/mol	NIST Webbook
hfus	13.56	kJ/mol	Joback Method
hvap	75.47	kJ/mol	Joback Method
log10ws	0.54		Crippen Method
logp	-1.030		Crippen Method

mcvol	98.920	ml/mol	McGowan Method
pc	5080.25	kPa	Joback Method
tb	587.11	K	Joback Method
tc	749.41	K	Joback Method
tf	470.00 ± 2.00	K	NIST Webbook
tf	473.70 ± 0.10	K	NIST Webbook
tf	471.30 ± 0.40	K	NIST Webbook
vc	0.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.16	J/mol×K	749.41	Joback Method
cpg	284.21	J/mol×K	695.31	Joback Method
cpg	278.31	J/mol×K	668.26	Joback Method
cpg	272.09	J/mol×K	641.21	Joback Method
cpg	265.56	J/mol×K	614.16	Joback Method
cpg	258.67	J/mol×K	587.11	Joback Method
cpg	289.82	J/mol×K	722.36	Joback Method
cps	182.60	J/mol×K	299.15	NIST Webbook
dvisc	0.0063873	Pa×s	373.68	Joback Method
dvisc	0.0011719	Pa×s	416.36	Joback Method
dvisc	0.0002947	Pa×s	459.05	Joback Method
dvisc	0.0000937	Pa×s	501.74	Joback Method
dvisc	0.0000357	Pa×s	544.42	Joback Method
dvisc	0.0539145	Pa×s	330.99	Joback Method
dvisc	0.0000156	Pa×s	587.11	Joback Method
hfust	5.38	kJ/mol	470.00	NIST Webbook
hfust	4.72	kJ/mol	474.40	NIST Webbook
hfust	5.38	kJ/mol	470.00	NIST Webbook
hfust	23.17	kJ/mol	354.00	NIST Webbook
hfust	4.70	kJ/mol	418.00	NIST Webbook
hfust	4.80	kJ/mol	472.40	NIST Webbook
sfust	11.44	J/mol×K	470.00	NIST Webbook
sfust	65.46	J/mol×K	354.00	NIST Webbook

Sources

Partial Molar Isentropic Compressions and Partial Molar Volumes of Selected Branched Aliphatic 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=C77850&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume