1,3-Pentanediol, 2,2,4-trimethyl-

Other names: 1,3-Dihydroxy-2,2,4-trimethyl pentane
2,2,4-Trimethyl pentanediol-1,3
2,2,4-Trimethyl-1,3-pentanediol
2,2,4-trimethylpentane-1,3-diol
TMPD
TMPD Glycol

Inchi: InChI=1S/C8H18O2/c1-6(2)7(10)8(3,4)5-9/h6-7,9-10H,5H2,1-4H3

InchiKey: JCTXKRPTIMZBJT-UHFFFAOYSA-N

Formula: C8H18O2

SMILES: CC(C)C(O)C(C)(C)CO

Mol. weight [g/mol]: 146.23

CAS: 144-19-4

Physical Properties

Property code	Value	Unit	Source
gf	-259.20	kJ/mol	Joback Method
hf	-532.22	kJ/mol	Joback Method
hfus	10.19	kJ/mol	Joback Method
hvap	64.69	kJ/mol	Joback Method
log10ws	-1.33		Crippen Method
logp	1.022		Crippen Method
mcvol	135.320	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
rinpol	1156.60		NIST Webbook
ripol	1980.00		NIST Webbook
ripol	1980.00		NIST Webbook
tb	505.20	K	NIST Webbook
tc	732.07	K	Joback Method
tf	323.15 ± 3.00	K	NIST Webbook
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	349.04	J/mol×K	562.69	Joback Method
cpg	360.14	J/mol×K	590.92	Joback Method
cpg	370.70	J/mol×K	619.15	Joback Method
cpg	380.75	J/mol×K	647.38	Joback Method
cpg	390.29	J/mol×K	675.61	Joback Method
cpg	399.36	J/mol×K	703.84	Joback Method
cpg	407.98	J/mol×K	732.07	Joback Method
dvisc	0.0000387	Pa×s	562.69	Joback Method
dvisc	0.0232070	Pa×s	322.10	Joback Method
dvisc	0.3212126	Pa×s	273.98	Joback Method
dvisc	0.0007427	Pa×s	418.33	Joback Method
dvisc	0.0002263	Pa×s	466.45	Joback Method
dvisc	0.0000861	Pa×s	514.57	Joback Method
dvisc	0.0033196	Pa×s	370.22	Joback Method
hfust	24.20	kJ/mol	328.30	NIST Webbook
hvapt	66.60 ± 2.10	kJ/mol	442.50	NIST Webbook
hvapt	60.30 ± 1.70	kJ/mol	442.50	NIST Webbook
hvapt	55.00 ± 1.60	kJ/mol	442.50	NIST Webbook
hvapt	58.50	kJ/mol	457.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63742e+01
Coeff. B	-4.97984e+03
Coeff. C	-8.15960e+01
Temperature range (K), min.	391.16
Temperature range (K), max.	531.74

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C144194&Units=SI

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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume