

# 2,4,4-Trimethyl-2,3-pentanediol

<b>Inchi:</b>	InChI=1S/C8H18O2/c1-7(2,3)6(9)8(4,5)10/h6,9-10H,1-5H3
<b>InchiKey:</b>	JDYWKAYETKZYIF-UHFFFAOYSA-N
<b>Formula:</b>	C8H18O2
<b>SMILES:</b>	CC(C)(C)C(O)C(C)(C)O
<b>Mol. weight [g/mol]:</b>	146.23
<b>CAS:</b>	64512-96-5

## Physical Properties

Property code	Value	Unit	Source
gf	-253.92	kJ/mol	Joback Method
hf	-535.69	kJ/mol	Joback Method
hfus	6.30	kJ/mol	Joback Method
hvap	63.78	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	1.164		Crippen Method
mcvol	135.320	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
tb	559.90	K	Joback Method
tc	734.73	K	Joback Method
tf	291.40	K	Joback Method
vc	0.493	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.11	J/molxK	559.90	Joback Method
cpg	363.56	J/molxK	589.04	Joback Method
cpg	374.36	J/molxK	618.18	Joback Method
cpg	384.55	J/molxK	647.31	Joback Method
cpg	394.16	J/molxK	676.45	Joback Method
cpg	403.23	J/molxK	705.59	Joback Method
cpg	411.79	J/molxK	734.73	Joback Method
dvisc	0.1508509	Paxs	291.40	Joback Method
dvisc	0.0152122	Paxs	336.15	Joback Method

dvisc	0.0026300	Paxs	380.90	Joback Method
dvisc	0.0006576	Paxs	425.65	Joback Method
dvisc	0.0002141	Paxs	470.40	Joback Method
dvisc	0.0000847	Paxs	515.15	Joback Method
dvisc	0.0000389	Paxs	559.90	Joback Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C64512965&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C64512965&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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