

# 1,3-Dioxane, 2,2,4,6-tetramethyl-, trans-

<b>Other names:</b>	m-Dioxane, 2,2,4,6-tetramethyl-, trans- trans-2,2,4,6-Tetramethyl-1,3-dioxane 2,2,cis-4,6-Tetramethyl-1,3-dioxane
<b>Inchi:</b>	InChI=1S/C8H16O2/c1-6-5-7(2)10-8(3,4)9-6/h6-7H,5H2,1-4H3/t6-,7-/m0/s1
<b>InchiKey:</b>	GPKRWHGIASNHBE-BQBZGAKWSA-N
<b>Formula:</b>	C8H16O2
<b>SMILES:</b>	CC1CC(C)OC(C)(C)O1
<b>Mol. weight [g/mol]:</b>	144.21
<b>CAS:</b>	20268-00-2

## Physical Properties

Property code	Value	Unit	Source
chl	-4908.40 ± 4.70	kJ/mol	NIST Webbook
gf	-152.22	kJ/mol	Joback Method
hf	-484.40 ± 4.90	kJ/mol	NIST Webbook
hf	-485.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-526.30 ± 4.70	kJ/mol	NIST Webbook
hfus	20.11	kJ/mol	Joback Method
hvap	41.90 ± 1.30	kJ/mol	NIST Webbook
log10ws	-2.07		Crippen Method
logp	1.936		Crippen Method
mcvol	124.460	ml/mol	McGowan Method
pc	3018.96	kPa	Joback Method
tb	384.65 ± 1.50	K	NIST Webbook
tc	655.64	K	Joback Method
tf	255.86	K	Joback Method
vc	0.455	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.84	J/molxK	446.79	Joback Method
cpg	295.30	J/molxK	481.60	Joback Method
cpg	311.72	J/molxK	516.41	Joback Method

cpg	327.19	J/mol×K	551.22	Joback Method
cpg	341.78	J/mol×K	586.02	Joback Method
cpg	355.58	J/mol×K	620.83	Joback Method
cpg	368.66	J/mol×K	655.64	Joback Method

## Sources

<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>
<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=C20268002&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C20268002&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfl:</b>	Liquid phase 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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