

# Oxirane, tetramethyl-

<b>Other names:</b>	Tetramethylethylene oxide Butane, 2,3-epoxy-2,3-dimethyl- Tetramethyloxirane 2,3-Dimethyl-2-butene oxide 2,3-Dimethyl-2,3-epoxybutane 2,3-Epoxy-2,3-dimethylbutane 2,2,3,3-Tetramethyl-oxirane
<b>Inchi:</b>	InChI=1S/C6H12O/c1-5(2)6(3,4)7-5/h1-4H3
<b>InchiKey:</b>	SYQIWVMFOAHDMK-UHFFFAOYSA-N
<b>Formula:</b>	C6H12O
<b>SMILES:</b>	CC1(C)OC1(C)C
<b>Mol. weight [g/mol]:</b>	100.16
<b>CAS:</b>	5076-20-0

## Physical Properties

Property code	Value	Unit	Source
gf	-44.42	kJ/mol	Joback Method
hf	-216.23	kJ/mol	Joback Method
hfus	5.88	kJ/mol	Joback Method
hvap	30.76	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.574		Crippen Method
mcvol	90.410	ml/mol	McGowan Method
pc	3829.28	kPa	Joback Method
rinpol	681.40		NIST Webbook
rinpol	682.20		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	681.40		NIST Webbook
rinpol	681.60		NIST Webbook
rinpol	681.90		NIST Webbook
tb	366.18	K	Joback Method
tc	562.99	K	Joback Method
tf	245.45	K	Joback Method
vc	0.344	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	170.49	J/mol×K	366.18	Joback Method
cpg	184.68	J/mol×K	398.98	Joback Method
cpg	197.46	J/mol×K	431.78	Joback Method
cpg	208.97	J/mol×K	464.58	Joback Method
cpg	219.37	J/mol×K	497.38	Joback Method
cpg	228.81	J/mol×K	530.19	Joback Method
cpg	237.44	J/mol×K	562.99	Joback Method

## Sources

<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=C5076200&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5076200&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<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>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>rinpol:</b>	Non-polar retention indices
<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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