

# Oxetane, 3,3-dimethyl-

<b>Other names:</b>	.beta.-.beta.'-dimethyltrimethylene oxide 1,3-Epoxy-2,2-dimethylpropane 3,3-Dimethyltrimethylene oxide 3,3-dimethyloxetane Propane, 1,3-epoxy-2,2-dimethyl- «beta», «beta»-Dimethyltrimethylene oxide
<b>Inchi:</b>	InChI=1S/C5H10O/c1-5(2)3-6-4-5/h3-4H2,1-2H3
<b>InchiKey:</b>	RVGLUKRYMXEQAH-UHFFFAOYSA-N
<b>Formula:</b>	C5H10O
<b>SMILES:</b>	CC1(C)COC1
<b>Mol. weight [g/mol]:</b>	86.13
<b>CAS:</b>	6921-35-3

## Physical Properties

Property code	Value	Unit	Source
chl	-3214.50 ± 1.60	kJ/mol	NIST Webbook
chl	-3140.20 ± 0.20	kJ/mol	NIST Webbook
gf	-51.74	kJ/mol	Joback Method
hf	-148.20 ± 1.70	kJ/mol	NIST Webbook
hfl	-182.20 ± 1.60	kJ/mol	NIST Webbook
hfus	6.42	kJ/mol	Joback Method
hvap	34.07	kJ/mol	NIST Webbook
hvap	33.90 ± 0.30	kJ/mol	NIST Webbook
hvap	34.00	kJ/mol	NIST Webbook
hvap	33.94 ± 0.29	kJ/mol	NIST Webbook
log10ws	-0.66		Crippen Method
logp	1.043		Crippen Method
mcvol	76.320	ml/mol	McGowan Method
pc	4403.25	kPa	Joback Method
rinpol	666.00		NIST Webbook
rinpol	648.00		NIST Webbook
tb	349.65 ± 2.00	K	NIST Webbook
tb	353.70	K	NIST Webbook

tb	352.80	K	Isobaric Vapor-Liquid Equilibrium for Two Binary Systems of 3,3-Dimethyloxetane + Methyl Cyclohexane and 3-Chloro-2,2-dimethyl-1-propanol + Methyl Cyclohexane at 101.3 kPa
tc	549.87	K	Joback Method
tf	211.00	K	Joback Method
vc	0.283	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.04	J/mol×K	483.91	Joback Method
cpg	185.06	J/mol×K	516.89	Joback Method
cpg	131.49	J/mol×K	352.00	Joback Method
cpg	144.07	J/mol×K	384.98	Joback Method
cpg	155.64	J/mol×K	417.96	Joback Method
cpg	166.26	J/mol×K	450.93	Joback Method
cpg	193.40	J/mol×K	549.87	Joback Method
hvapt	30.85	kJ/mol	353.70	NIST Webbook
pvap	101.30	kPa	352.80	Isobaric Vapor-Liquid Equilibrium for Two Binary Systems of 3,3-Dimethyloxetane + Methyl Cyclohexane and 3-Chloro-2,2-dimethyl-1-propanol + Methyl Cyclohexane at 101.3 kPa

## Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

Isobaric Vapor-Liquid Equilibrium for Two Binary Systems of Joback Method

<https://www.doi.org/10.1021/acs.jced.8b00966>

McGowan Method:

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

3-Chloro-2,2-dimethyl-1-propanol + Methyl Cyclohexane at 101.3 kPa: NIST Webbook

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C6921353&Units=SI>

# 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>hvapt:</b>	Enthalpy of vaporization at a given temperature
<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>pvap:</b>	Vapor 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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