

# Cyclopentane, 1,1,3-trimethyl-

<b>Other names:</b>	1,1,3-Trimethylcyclopentane
<b>Inchi:</b>	InChI=1S/C8H16/c1-7-4-5-8(2,3)6-7/h7H,4-6H2,1-3H3
<b>InchiKey:</b>	OBKHYUIZSOIEPG-UHFFFAOYSA-N
<b>Formula:</b>	C8H16
<b>SMILES:</b>	CC1CCC(C)(C)C1
<b>Mol. weight [g/mol]:</b>	112.21
<b>CAS:</b>	4516-69-2

## Physical Properties

Property code	Value	Unit	Source
gf	39.83	kJ/mol	Joback Method
hf	-153.07	kJ/mol	Joback Method
hfus	5.18	kJ/mol	Joback Method
hvap	36.00	kJ/mol	NIST Webbook
log10ws	-4.48		Aqueous Solubility Prediction Method
logp	2.833		Crippen Method
mcvol	112.720	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
rinpol	725.70		NIST Webbook
rinpol	723.00		NIST Webbook
rinpol	725.10		NIST Webbook
rinpol	722.00		NIST Webbook
rinpol	719.00		NIST Webbook
rinpol	720.42		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	714.00		NIST Webbook
rinpol	719.00		NIST Webbook
rinpol	723.10		NIST Webbook
rinpol	727.10		NIST Webbook
rinpol	723.00		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	721.80		NIST Webbook
rinpol	723.70		NIST Webbook
rinpol	714.00		NIST Webbook
rinpol	727.50		NIST Webbook

rinpol	723.70	NIST Webbook
rinpol	719.00	NIST Webbook
rinpol	721.00	NIST Webbook
rinpol	723.00	NIST Webbook
rinpol	725.00	NIST Webbook
rinpol	727.00	NIST Webbook
rinpol	729.00	NIST Webbook
rinpol	726.00	NIST Webbook
rinpol	726.10	NIST Webbook
rinpol	724.00	NIST Webbook
rinpol	724.00	NIST Webbook
rinpol	724.00	NIST Webbook
rinpol	725.50	NIST Webbook
rinpol	724.80	NIST Webbook
rinpol	736.00	NIST Webbook
rinpol	724.00	NIST Webbook
rinpol	728.00	NIST Webbook
rinpol	720.00	NIST Webbook
rinpol	722.00	NIST Webbook
rinpol	724.00	NIST Webbook
rinpol	726.00	NIST Webbook
rinpol	728.00	NIST Webbook
rinpol	724.60	NIST Webbook
rinpol	728.00	NIST Webbook
rinpol	720.00	NIST Webbook
rinpol	740.00	NIST Webbook
rinpol	720.00	NIST Webbook
rinpol	724.00	NIST Webbook
rinpol	727.00	NIST Webbook
rinpol	731.00	NIST Webbook
rinpol	728.00	NIST Webbook
rinpol	720.42	NIST Webbook
rinpol	723.00	NIST Webbook
rinpol	723.10	NIST Webbook
rinpol	718.58	NIST Webbook
rinpol	721.60	NIST Webbook
rinpol	719.32	NIST Webbook
rinpol	719.35	NIST Webbook
rinpol	719.00	NIST Webbook
rinpol	722.00	NIST Webbook
rinpol	724.00	NIST Webbook
rinpol	733.00	NIST Webbook
rinpol	722.00	NIST Webbook
rinpol	727.00	NIST Webbook

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rinpol	726.00		NIST Webbook
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rinpol	740.00		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	722.70		NIST Webbook
rinpol	723.60		NIST Webbook
rinpol	725.10		NIST Webbook
rinpol	726.30		NIST Webbook
rinpol	727.40		NIST Webbook
rinpol	728.40		NIST Webbook
rinpol	722.00		NIST Webbook
rinpol	723.00		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	727.00		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	719.00		NIST Webbook
rinpol	720.00		NIST Webbook
tb	378.04	K	KDB
tc	594.34	K	Joback Method
tf	130.71 ± 0.12	K	NIST Webbook
tf	130.69 ± 0.20	K	NIST Webbook
tf	130.77 ± 0.20	K	NIST Webbook
tf	130.95	K	Aqueous Solubility Prediction Method
tf	130.69 ± 0.15	K	NIST Webbook
tf	130.71 ± 0.15	K	NIST Webbook
vc	0.421	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.45	J/mol×K	393.29	Joback Method
cpg	232.08	J/mol×K	426.80	Joback Method
cpg	248.56	J/mol×K	460.31	Joback Method
cpg	263.98	J/mol×K	493.81	Joback Method
cpg	278.43	J/mol×K	527.32	Joback Method
cpg	292.00	J/mol×K	560.83	Joback Method
cpg	304.76	J/mol×K	594.34	Joback Method

## Sources

<b>KDB:</b>	<a href="https://www.therc.org/research/kdb/hcprop/showprop.php?cmpid=488">https://www.therc.org/research/kdb/hcprop/showprop.php?cmpid=488</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</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=C4516692&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4516692&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
<b>KDB Vapor Pressure Data:</b>	<a href="https://www.therc.org/research/kdb/hcprop/showprop.php?cmpid=488">https://www.therc.org/research/kdb/hcprop/showprop.php?cmpid=488</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>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>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>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>rinpola:</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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