

# 3,4-Dimethylcyclohexanol

<b>Other names:</b>	3,4-dimethylcyclohexan-1-ol Cyclohexanol, 3,4-dimethyl-
<b>Inchi:</b>	InChI=1S/C8H16O/c1-6-3-4-8(9)5-7(6)2/h6-9H,3-5H2,1-2H3
<b>InchiKey:</b>	ZBAXJUPCYVIBSP-UHFFFAOYSA-N
<b>Formula:</b>	C8H16O
<b>SMILES:</b>	CC1CCC(O)CC1C
<b>Mol. weight [g/mol]:</b>	128.21
<b>CAS:</b>	5715-23-1

## Physical Properties

Property code	Value	Unit	Source
gf	-111.31	kJ/mol	Joback Method
hf	-347.04	kJ/mol	Joback Method
hfus	14.54	kJ/mol	Joback Method
hvap	49.89	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.803		Crippen Method
mcvol	118.590	ml/mol	McGowan Method
pc	3246.73	kPa	Joback Method
rinpola	1126.00		NIST Webbook
tb	462.20	K	NIST Webbook
tb	461.40 ± 3.00	K	NIST Webbook
tc	674.82	K	Joback Method
tf	239.64	K	Joback Method
vc	0.433	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.01	J/mol×K	484.83	Joback Method
cpg	291.52	J/mol×K	516.49	Joback Method
cpg	306.35	J/mol×K	548.16	Joback Method
cpg	320.50	J/mol×K	579.82	Joback Method
cpg	334.00	J/mol×K	611.49	Joback Method

cpg	346.84	J/mol×K	643.15	Joback Method
cpg	359.03	J/mol×K	674.82	Joback Method
dvisc	0.0327662	Paxs	239.64	Joback Method
dvisc	0.0075606	Paxs	280.50	Joback Method
dvisc	0.0025331	Paxs	321.37	Joback Method
dvisc	0.0010862	Paxs	362.24	Joback Method
dvisc	0.0005530	Paxs	403.10	Joback Method
dvisc	0.0003188	Paxs	443.97	Joback Method
dvisc	0.0002017	Paxs	484.83	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.61057e+01
Coeff. B	-4.50961e+03
Coeff. C	-6.96280e+01
Temperature range (K), min.	354.72
Temperature range (K), max.	487.41

## Sources

The Yaws Handbook of Vapor Pressure:  
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>  
<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

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

Joback Method:

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

McGowan Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C5715231&Units=SI>

## Legend

**cpg:** Ideal gas heat capacity  
**dvisc:** Dynamic viscosity  
**gf:** Standard Gibbs free energy of formation  
**hf:** 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>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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