

# 1-Pentyn-3-ol, 3,4-dimethyl-

<b>Other names:</b>	3,4-Dimethyl-1-penten-3-ol 3,4-Dimethyl-1-pentyn-3-ol
<b>Inchi:</b>	InChI=1S/C7H12O/c1-5-7(4,8)6(2)3/h1,6,8H,2-4H3
<b>InchiKey:</b>	DZNLEQBXXLGELU-UHFFFAOYSA-N
<b>Formula:</b>	C7H12O
<b>SMILES:</b>	C#CC(C)(O)C(C)C
<b>Mol. weight [g/mol]:</b>	112.17
<b>CAS:</b>	1482-15-1

## Physical Properties

Property code	Value	Unit	Source
gf	94.71	kJ/mol	Joback Method
hf	-62.17	kJ/mol	Joback Method
hfus	10.01	kJ/mol	Joback Method
hvap	46.03	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	1.027		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3796.32	kPa	Joback Method
tb	438.19	K	Joback Method
tc	623.88	K	Joback Method
tf	263.86	K	Joback Method
vc	0.392	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.23	J/mol×K	438.19	Joback Method
cpg	231.76	J/mol×K	469.14	Joback Method
cpg	241.68	J/mol×K	500.09	Joback Method
cpg	251.02	J/mol×K	531.04	Joback Method
cpg	259.82	J/mol×K	561.99	Joback Method
cpg	268.10	J/mol×K	592.93	Joback Method
cpg	275.90	J/mol×K	623.88	Joback Method

# Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.64196e+01
Coeff. B	-4.55664e+03
Coeff. C	-6.71610e+01
Temperature range (K), min.	349.15
Temperature range (K), max.	477.15

## Sources

<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>
<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=C1482151&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1482151&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>

## 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>pvap:</b>	Vapor pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

**tf:** Normal melting (fusion) point

**vc:** Critical Volume

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