

# 2-Pentyn-1-ol

<b>Other names:</b>	pent-2-yn-1-ol
<b>Inchi:</b>	InChI=1S/C5H8O/c1-2-3-4-5-6/h6H,2,5H2,1H3
<b>InchiKey:</b>	WLPYSOCRPHITDZ-UHFFFAOYSA-N
<b>Formula:</b>	C5H8O
<b>SMILES:</b>	CCC#CCO
<b>Mol. weight [g/mol]:</b>	84.12
<b>CAS:</b>	6261-22-9

## Physical Properties

Property code	Value	Unit	Source
gf	57.20	kJ/mol	Joback Method
hf	-26.46	kJ/mol	Joback Method
hfus	15.92	kJ/mol	Joback Method
hvap	45.55	kJ/mol	Joback Method
log10ws	-0.97		Crippen Method
logp	0.392		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	4782.59	kPa	Joback Method
tb	414.98	K	Joback Method
tc	599.21	K	Joback Method
tf	313.03	K	Joback Method
vc	0.296	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	142.38	J/molxK	414.98	Joback Method
cpg	149.23	J/molxK	445.68	Joback Method
cpg	155.82	J/molxK	476.39	Joback Method
cpg	162.17	J/molxK	507.09	Joback Method
cpg	168.26	J/molxK	537.80	Joback Method
cpg	174.12	J/molxK	568.50	Joback Method
cpg	179.75	J/molxK	599.21	Joback Method

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	357.70	K	7.60	NIST Webbook
tbrp	334.50 ± 0.50	K	2.00	NIST Webbook
tbrp	334.70	K	2.00	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.64795e+01
Coeff. B	-4.10284e+03
Coeff. C	-5.16780e+01
Temperature range (K), min.	305.15
Temperature range (K), max.	419.15

## Sources

The Yaws Handbook of Vapor

Pressure:

Crippen Method:

Crippen Method:

Joback Method:

McGowan Method:

NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

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

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

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C6261229&Units=SI>

## Legend

**cpg:** Ideal gas heat capacity

**gf:** 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>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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