

# pent-4-enenitrile

<b>Other names:</b>	4-pentenitrile But-3-enyl cyanide
<b>Inchi:</b>	InChI=1S/C5H7N/c1-2-3-4-5-6/h2H,1,3-4H2
<b>InchiKey:</b>	CFEYBLWMNFZOPB-UHFFFAOYSA-N
<b>Formula:</b>	C5H7N
<b>SMILES:</b>	C=CCCC#N
<b>Mol. weight [g/mol]:</b>	81.12
<b>CAS:</b>	592-51-8

## Physical Properties

Property code	Value	Unit	Source
gf	212.24	kJ/mol	Joback Method
hf	143.78	kJ/mol	Joback Method
hfus	8.93	kJ/mol	Joback Method
hvap	36.53	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.476		Crippen Method
mcvol	78.390	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
rinpol	742.00		NIST Webbook
rinpol	742.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	731.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	735.00		NIST Webbook
ripol	1275.00		NIST Webbook
ripol	1275.00		NIST Webbook
ripol	1244.00		NIST Webbook
ripol	1275.00		NIST Webbook
ripol	1244.00		NIST Webbook
tb	413.20	K	NIST Webbook
tc	607.39	K	Joback Method
tf	209.34	K	Joback Method
vc	0.323	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.04	J/mol×K	412.56	Joback Method
cpg	145.20	J/mol×K	445.03	Joback Method
cpg	152.02	J/mol×K	477.50	Joback Method
cpg	158.51	J/mol×K	509.97	Joback Method
cpg	164.69	J/mol×K	542.44	Joback Method
cpg	170.57	J/mol×K	574.91	Joback Method
cpg	176.15	J/mol×K	607.39	Joback Method

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	333.70	K	5.30	NIST Webbook

# Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.46534e+01
Coeff. B	-3.58448e+03
Coeff. C	-5.60060e+01
Temperature range (K), min.	305.52
Temperature range (K), max.	439.70

# Sources

**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=C592518&Units=SI>

**The Yaws Handbook of Vapor Pressure:**

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

**Crippen Method:**

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

**Crippen Method:**

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

## 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>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<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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