

# (Z)-pent-2-enenitrile

Other names:	(Z)-2-Pentenitrile
Inchi:	InChI=1S/C5H7N/c1-2-3-4-5-6/h3-4H,2H2,1H3/b4-3-
InchiKey:	ISBHMJZRKAFTGE-ARJAWSKDSA-N
Formula:	C5H7N
SMILES:	CCC=CC#N
Mol. weight [g/mol]:	81.12
CAS:	25899-50-7

## Physical Properties

Property code	Value	Unit	Source
chl	-3039.80 ± 1.20	kJ/mol	NIST Webbook
gf	204.62	kJ/mol	Joback Method
hf	115.00 ± 1.20	kJ/mol	NIST Webbook
hfl	71.80 ± 1.20	kJ/mol	NIST Webbook
hfus	10.41	kJ/mol	Joback Method
hvap	43.20	kJ/mol	NIST Webbook
hvap	43.20 ± 0.20	kJ/mol	NIST Webbook
hvap	43.20	kJ/mol	NIST Webbook
log10ws	-1.64		Crippen Method
logp	1.476		Crippen Method
mcvol	78.390	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
tb	420.04	K	Joback Method
tc	620.58	K	Joback Method
tf	206.02	K	Joback Method
vc	0.322	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.82	J/molxK	420.04	Joback Method
cpg	144.23	J/molxK	453.46	Joback Method
cpg	151.25	J/molxK	486.89	Joback Method
cpg	157.88	J/molxK	520.31	Joback Method

cpg	164.16	J/mol×K	553.73	Joback Method
cpg	170.09	J/mol×K	587.15	Joback Method
cpg	175.70	J/mol×K	620.58	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	332.70	K	9.60	NIST Webbook

## Sources

Joback Method:	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C25899507&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C25899507&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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