

# n-Pentylmalononitrile

<b>Inchi:</b>	InChI=1S/C8H12N2/c1-2-3-4-5-8(6-9)7-10/h8H,2-5H2,1H3
<b>InchiKey:</b>	HMPREYSQSBVPJ-UHFFFAOYSA-N
<b>Formula:</b>	C8H12N2
<b>SMILES:</b>	CCCCC(C#N)C#N
<b>Mol. weight [g/mol]:</b>	136.19
<b>CAS:</b>	42046-61-7

## Physical Properties

Property code	Value	Unit	Source
chl	-4931.76 ± 0.50	kJ/mol	NIST Webbook
gf	280.40	kJ/mol	Joback Method
hf	135.80 ± 0.63	kJ/mol	NIST Webbook
hfl	68.74 ± 0.50	kJ/mol	NIST Webbook
hfus	15.96	kJ/mol	Joback Method
hvap	67.10	kJ/mol	NIST Webbook
hvap	67.00 ± 0.40	kJ/mol	NIST Webbook
log10ws	-2.66		Crippen Method
logp	2.230		Crippen Method
mcvol	126.340	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
tb	586.16	K	Joback Method
tc	792.14	K	Joback Method
tf	294.90	K	Joback Method
vc	0.529	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.81	J/mol×K	586.16	Joback Method
cpg	305.81	J/mol×K	620.49	Joback Method
cpg	315.29	J/mol×K	654.82	Joback Method
cpg	324.27	J/mol×K	689.15	Joback Method
cpg	332.76	J/mol×K	723.48	Joback Method
cpg	340.78	J/mol×K	757.81	Joback Method

cpg	348.36	J/mol×K	792.14	Joback Method
hvapt	66.90 ± 0.40	kJ/mol	313.00	NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C42046617&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C42046617&amp;Units=SI</a>
<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>

## Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<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>hfl:</b>	Liquid phase 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>hvapt:</b>	Enthalpy of vaporization at a given temperature
<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>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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