

# 3-methyl-2-butenenitrile

<b>Other names:</b>	Senecionitrile
<b>Inchi:</b>	InChI=1S/C5H7N/c1-5(2)3-4-6/h3H,1-2H3
<b>InchiKey:</b>	AUGKLUNRHYPDAM-UHFFFAOYSA-N
<b>Formula:</b>	C5H7N
<b>SMILES:</b>	CC(C)=CC#N
<b>Mol. weight [g/mol]:</b>	81.12
<b>CAS:</b>	4786-24-7

## Physical Properties

Property code	Value	Unit	Source
gf	196.07	kJ/mol	Joback Method
hf	125.78	kJ/mol	Joback Method
hfus	9.10	kJ/mol	Joback Method
hvap	37.24	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.476		Crippen Method
mcvol	78.390	ml/mol	McGowan Method
pc	3602.88	kPa	Joback Method
rinpol	770.00		NIST Webbook
rinpol	770.00		NIST Webbook
tb	419.92	K	Joback Method
tc	624.57	K	Joback Method
tf	192.06	K	Joback Method
vc	0.323	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.79	J/molxK	419.92	Joback Method
cpg	144.32	J/molxK	454.03	Joback Method
cpg	151.44	J/molxK	488.14	Joback Method
cpg	158.15	J/molxK	522.25	Joback Method
cpg	164.50	J/molxK	556.36	Joback Method
cpg	170.49	J/molxK	590.47	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4786247&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4786247&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>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>rinpol:</b>	Non-polar retention indices
<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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