

# Butanenireile, 2-methoxy

<b>Inchi:</b>	InChI=1S/C5H9NO/c1-3-5(4-6)7-2/h5H,3H2,1-2H3
<b>InchiKey:</b>	HLGNKWWNJVVYHJO-UHFFFAOYSA-N
<b>Formula:</b>	C5H9NO
<b>SMILES:</b>	CCC(C#N)OC
<b>Mol. weight [g/mol]:</b>	99.13

## Physical Properties

Property code	Value	Unit	Source
gf	16.96	kJ/mol	Joback Method
hf	-119.15	kJ/mol	Joback Method
hfus	7.88	kJ/mol	Joback Method
hvap	39.22	kJ/mol	Joback Method
log10ws	-0.98		Crippen Method
logp	0.935		Crippen Method
mcvol	88.560	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
rinpol	854.00		NIST Webbook
tb	437.86	K	Joback Method
tc	632.31	K	Joback Method
tf	218.33	K	Joback Method
vc	0.353	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.10	J/molxK	437.86	Joback Method
cpg	181.16	J/molxK	470.27	Joback Method
cpg	188.95	J/molxK	502.68	Joback Method
cpg	196.47	J/molxK	535.08	Joback Method
cpg	203.72	J/molxK	567.49	Joback Method
cpg	210.69	J/molxK	599.90	Joback Method
cpg	217.38	J/molxK	632.31	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R511412&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R511412&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>hvac:</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>mccol:</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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