

# Nonanoic acid, 2-cyanoethyl ester

<b>Inchi:</b>	InChI=1S/C12H21NO2/c1-2-3-4-5-6-7-9-12(14)15-11-8-10-13/h2-9,11H2,1H3
<b>InchiKey:</b>	MCQNPEQSCWSQAE-UHFFFAOYSA-N
<b>Formula:</b>	C12H21NO2
<b>SMILES:</b>	CCCCCCCCC(=O)OCCC#N
<b>Mol. weight [g/mol]:</b>	211.30

## Physical Properties

Property code	Value	Unit	Source
gf	-50.58	kJ/mol	Joback Method
hf	-370.93	kJ/mol	Joback Method
hfus	31.13	kJ/mol	Joback Method
hvap	61.94	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.194		Crippen Method
mcvol	188.760	ml/mol	McGowan Method
pc	1812.32	kPa	Joback Method
tb	652.33	K	Joback Method
tc	837.17	K	Joback Method
tf	362.15	K	Joback Method
vc	0.757	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.75	J/molxK	652.33	Joback Method
cpg	517.43	J/molxK	683.14	Joback Method
cpg	530.47	J/molxK	713.94	Joback Method
cpg	542.86	J/molxK	744.75	Joback Method
cpg	554.63	J/molxK	775.56	Joback Method
cpg	565.78	J/molxK	806.36	Joback Method
cpg	576.33	J/molxK	837.17	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=B6009694&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009694&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>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>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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