

# Ethanol, 2-(2-cyanoethyl) ether

<b>Inchi:</b>	InChI=1S/C6H10O2/c1-2-3-5-8-6-4-7/h1,7H,3-6H2
<b>InchiKey:</b>	AMRBGANUAYUVFH-UHFFFAOYSA-N
<b>Formula:</b>	C6H10O2
<b>SMILES:</b>	C#CCCOCCO
<b>Mol. weight [g/mol]:</b>	114.14

## Physical Properties

Property code	Value	Unit	Source
gf	-19.11	kJ/mol	Joback Method
hf	-159.72	kJ/mol	Joback Method
hfus	19.55	kJ/mol	Joback Method
hvap	47.90	kJ/mol	Joback Method
log10ws	-0.48		Crippen Method
logp	0.019		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	4051.80	kPa	Joback Method
rinpola	866.00		NIST Webbook
tb	441.40	K	Joback Method
tc	613.14	K	Joback Method
tf	287.40	K	Joback Method
vc	0.370	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.37	J/mol×K	441.40	Joback Method
cpg	209.19	J/mol×K	470.02	Joback Method
cpg	216.72	J/mol×K	498.65	Joback Method
cpg	223.98	J/mol×K	527.27	Joback Method
cpg	230.97	J/mol×K	555.89	Joback Method
cpg	237.70	J/mol×K	584.52	Joback Method
cpg	244.16	J/mol×K	613.14	Joback Method

# Sources

<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=R511625&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R511625&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

# 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>rinpola:</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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