

# Ethyl cyanoacetate

<b>Other names:</b>	Acetic acid, 2-cyano-, ethyl ester Acetic acid, cyano-, ethyl ester Cyanacetate ethyle Cyanoacetic acid, ethyl ester Cyanoacetic ester Esteri cianoacetico Ethyl cyanacetate Ethyl ester of cyanoacetic acid Ethylester kyseliny kyanoctove Malonic acid, ethyl ester nitrile NCCH <sub>2</sub> COOC <sub>2</sub> H <sub>5</sub> NSC 8844 UN 2666 USAF KF-25 ethyl 2-cyanoacetate ethyl cyanoethanoate
<b>Inchi:</b>	InChI=1S/C5H7NO2/c1-2-8-5(7)3-4-6/h2-3H2,1H3
<b>InchiKey:</b>	ZIUSEGSNTOUIPT-UHFFFAOYSA-N
<b>Formula:</b>	C <sub>5</sub> H <sub>7</sub> NO <sub>2</sub>
<b>SMILES:</b>	CCOC(=O)CC#N
<b>Mol. weight [g/mol]:</b>	113.11
<b>CAS:</b>	105-56-6

## Physical Properties

Property code	Value	Unit	Source
chl	-2638.00	kJ/mol	NIST Webbook
gf	-109.52	kJ/mol	Joback Method
hf	-226.45	kJ/mol	Joback Method
hfl	-330.30	kJ/mol	NIST Webbook
hfus	13.00	kJ/mol	Joback Method
hvap	46.36	kJ/mol	Joback Method
log10ws	-0.64		Crippen Method
logp	0.463		Crippen Method
mvol	90.130	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
rinpol	962.00		NIST Webbook
rinpol	962.00		NIST Webbook

rinpol	960.00		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	959.00		NIST Webbook
sl	177.45	J/molxK	NIST Webbook
sl	275.33	J/molxK	NIST Webbook
tb	482.20	K	NIST Webbook
tc	692.81	K	Joback Method
tf	371.65 ± 1.50	K	NIST Webbook
tt	160.00 ± 1.00	K	NIST Webbook
tt	246.80 ± 0.10	K	NIST Webbook
tt	247.00 ± 1.00	K	NIST Webbook
vc	0.365	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.49	J/molxK	659.37	Joback Method
cpg	203.97	J/molxK	592.49	Joback Method
cpg	210.38	J/molxK	625.93	Joback Method
cpg	222.32	J/molxK	692.81	Joback Method
cpg	183.09	J/molxK	492.17	Joback Method
cpg	190.32	J/molxK	525.61	Joback Method
cpg	197.29	J/molxK	559.05	Joback Method
cpl	220.22	J/molxK	298.15	NIST Webbook
cpl	222.04	J/molxK	300.00	NIST Webbook
dvisc	0.0019618	Paxs	308.15	Volumetric and Transport Properties of Binary Liquid Mixtures of Phenylacetonitrile with Aliphatic Esters at Temperatures of (303.15 to 313.15) K
dvisc	0.0017698	Paxs	313.15	Volumetric and Transport Properties of Binary Liquid Mixtures of Phenylacetonitrile with Aliphatic Esters at Temperatures of (303.15 to 313.15) K

dvisc	0.0021861	Paxs	303.15	Volumetric and Transport Properties of Binary Liquid Mixtures of Phenylacetonitrile with Aliphatic Esters at Temperatures of (303.15 to 313.15) K
hfust	11.78	kJ/mol	246.80	NIST Webbook
hfust	11.78	kJ/mol	246.80	NIST Webbook
hvapt	66.90	kJ/mol	409.50	NIST Webbook
speedsl	1359.00	m/s	318.15	Density and Speed of Sound of Binary Mixtures of N-Methylacetamide with Ethyl Acetate, Ethyl Chloroacetate, and Ethyl Cyanoacetate in the Temperature Interval (303.15 to 318.15) K
speedsl	1368.00	m/s	313.15	Density and Speed of Sound of Binary Mixtures of N-Methylacetamide with Ethyl Acetate, Ethyl Chloroacetate, and Ethyl Cyanoacetate in the Temperature Interval (303.15 to 318.15) K
speedsl	1385.00	m/s	308.15	Density and Speed of Sound of Binary Mixtures of N-Methylacetamide with Ethyl Acetate, Ethyl Chloroacetate, and Ethyl Cyanoacetate in the Temperature Interval (303.15 to 318.15) K

speedsl	1397.00	m/s	303.15	Density and Speed of Sound of Binary Mixtures of N-Methylacetamide with Ethyl Acetate, Ethyl Chloroacetate, and Ethyl Cyanoacetate in the Temperature Interval (303.15 to 318.15) K
---------	---------	-----	--------	---

## 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=C105566&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C105566&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>Density and Speed of Sound of Binary Mixtures of N-Methylacetamide with Ethyl Acetate, Ethyl Chloroacetate, and Ethyl Cyanoacetate in the Temperature Interval (303.15 to 318.15) K:</b>	<a href="https://www.doi.org/10.1021/je060343y">https://www.doi.org/10.1021/je060343y</a>
<b>Polymers and Their Properties and Binary Liquid Mixtures of Polyacrylonitrile with Aliphatic Esters at Temperatures of (303.15 to 313.15) K:</b>	<a href="https://www.doi.org/10.1021/je900525f">https://www.doi.org/10.1021/je900525f</a>

## Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>cpl:</b>	Liquid phase heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>hfust:</b>	Enthalpy of fusion at a given temperature
<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>rinpol:</b>	Non-polar retention indices

<b>sl:</b>	Liquid phase molar entropy at standard conditions
<b>speedsl:</b>	Speed of sound in fluid
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>tt:</b>	Triple Point Temperature
<b>vc:</b>	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/35-965-2/Ethyl-cyanoacetate.pdf>

Generated by Cheméo on 2025-01-27 04:18:41.424158477 +0000 UTC m=+1159737.271084095.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.