Ethyl cyanoacetate

Other names:	Acetic acid, 2-cyano-, ethyl ester
	Acetic acid, cyano-, ethyl ester
	Cyanacetate ethyle
	Cyanoacetic acid, ethyl ester
	Cyanoacetic ester
	Estere cianoacetico
	Ethyl cyanacetate
	Ethyl ester of cyanoacetic acid
	Ethylester kyseliny kyanoctove
	Malonic acid, ethyl ester nitrile
	NCCH2COOC2H5
	NSC 8844
	UN 2666
	USAF KF-25
	ethyl 2-cyanoacetate
	ethyl cyanoethanoate
Inchi:	InChI=1S/C5H7NO2/c1-2-8-5(7)3-4-6/h2-3H2,1H3
InchiKey:	ZIUSEGSNTOUIPT-UHFFFAOYSA-N
Formula:	C5H7NO2
SMILES:	CCOC(=O)CC#N
Mol. weight [g/mol]:	113.11
CAS:	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
mcvol	90.130	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
rinpol	962.00		NIST Webbook
rinpol	959.00		NIST Webbook

rinpol	962.00		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	960.00		NIST Webbook
sl	275.33	J/mol×K	NIST Webbook
sl	177.45	J/mol×K	NIST Webbook
tb	482.20	K	NIST Webbook
tc	692.81	K	Joback Method
tf	371.65 ± 1.50	K	NIST Webbook
tt	247.00 ± 1.00	K	NIST Webbook
tt	160.00 ± 1.00	K	NIST Webbook
tt	246.80 ± 0.10	K	NIST Webbook
vc	0.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.32	J/mol×K	692.81	Joback Method
cpg	183.09	J/mol×K	492.17	Joback Method
cpg	216.49	J/mol×K	659.37	Joback Method
cpg	210.38	J/mol×K	625.93	Joback Method
cpg	203.97	J/mol×K	592.49	Joback Method
cpg	197.29	J/mol×K	559.05	Joback Method
cpg	190.32	J/mol×K	525.61	Joback Method
cpl	220.22	J/mol×K	298.15	NIST Webbook
cpl	222.04	J/mol×K	300.00	NIST Webbook
dvisc	0.0017698	Pa×s	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	0.0019618	Pa×s	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	0.0021861	Pa×s	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	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
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	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	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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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:	https://www.doi.org/10.1021/je060343y
Volumetric and Thermodynamic Properties of Binary Liquid Mixtures of Joback Method:	https://www.doi.org/10.1021/je900525f
	https://en.wikipedia.org/wiki/Joback_method
Nitrile with Aliphatic Esters at Temperatures of (303.15 to 313.15) K: McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C105566&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices

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