2-Propenoic acid, ethyl ester

Other names:	Acrylate d'ethyle
	Acrylic acid ethyl ester
	Acrylic acid, ethyl ester (inhibited)
	Acrylsaeureaethylester
	Aethylacrylat
	Akrylanem etylu
	CH2=CHCOOC2H5
	Carboset 511
	ETHYL PROPENOATE
	Ethoxycarbonylethylene
	Ethyl 2-propenoate
	Ethyl acrylate
	Ethyl acrylate, inhibited
	Ethyl ester of 2-propenoic acid
	Ethylacrylaat
	Ethylakrylat
	Ethylester kyseliny akrylove
	Etil acrilato
	Etilacrilatului
	NCI-C50384
	NSC 8263
	Rcra waste number U113
	acrylic acid, ethyl ester
	propenoic acid, ethyl ester
Inchi:	InChI=1S/C5H8O2/c1-3-5(6)7-4-2/h3H,1,4H2,2H3
InchiKey:	JIGUQPWFLRLWPJ-UHFFFAOYSA-N
Formula:	C5H8O2
SMILES:	C=CC(=O)OCC
Mol. weight [g/mol]:	100.12
CAS:	140-88-5

Physical Properties

Property code	Value	Unit	Source
af	0.4000		KDB
chl	-2715.00	kJ/mol	NIST Webbook
gf	-154.86	kJ/mol	Joback Method

hf	-327.80	kJ/mol	NIST Webbook
hf	-331.40	kJ/mol	NIST Webbook
hf	-354.20	kJ/mol	NIST Webbook
hfl	-370.60	kJ/mol	NIST Webbook
hfl	-393.40	kJ/mol	NIST Webbook
hfl	-367.00	kJ/mol	NIST Webbook
hfus	10.21	kJ/mol	Joback Method
hvap	39.20	kJ/mol	NIST Webbook
hvap	39.20	kJ/mol	NIST Webbook
ie	10.30	eV	NIST Webbook
log10ws	-0.74		Aqueous Solubility Prediction Method
logp	0.735		Crippen Method
mcvol	84.450	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
nfpas	%!d(float64=2)		KDB
pc	3740.00	kPa	KDB
rinpol	681.00		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	664.00		NIST Webbook
rinpol	702.00		NIST Webbook
rinpol	677.00		NIST Webbook
rinpol	664.00		NIST Webbook
rinpol	664.00		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	681.00		NIST Webbook
rinpol	648.00		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	676.00		NIST Webbook
rinpol	644.00		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	676.00		NIST Webbook
rinpol	648.00		NIST Webbook
rinpol	681.00		NIST Webbook
rinpol	680.00		NIST Webbook
rinpol	676.00		NIST Webbook
rinpol	644.00		NIST Webbook
rinpol	678.00		NIST Webbook
ripol	989.00		NIST Webbook
ripol	993.00		NIST Webbook
ripol	992.00		NIST Webbook
ripol	992.00		NIST Webbook
ripol	980.00		NIST Webbook
tb	372.50 ± 3.00	K	NIST Webbook

tb	372.75	K	NIST Webbook
tb	373.00	K	NIST Webbook
tb	373.00	K	NIST Webbook
tb	373.00	K	KDB
tc	552.00	K	KDB
tf	201.00	K	KDB
tf	201.15	K	NIST Webbook
tf	202.10	K	Aqueous Solubility Prediction Method
vc	0.320	m3/kmol	KDB
zc	0.2607630		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.35	J/mol×K	386.77	Joback Method
cpg	157.10	J/mol×K	417.17	Joback Method
cpg	164.59	J/mol×K	447.57	Joback Method
cpg	171.82	J/mol×K	477.97	Joback Method
cpg	178.80	J/mol×K	508.37	Joback Method
cpg	185.52	J/mol×K	538.77	Joback Method
cpg	191.98	J/mol×K	569.17	Joback Method
dvisc	0.0002673	Pa×s	386.77	Joback Method
dvisc	0.0013568	Pa×s	244.89	Joback Method
dvisc	0.0024241	Pa×s	216.51	Joback Method
dvisc	0.0005898	Pa×s	301.64	Joback Method
dvisc	0.0004330	Pa×s	330.02	Joback Method
dvisc	0.0003338	Pa×s	358.39	Joback Method
dvisc	0.0008567	Pa×s	273.26	Joback Method
hvapt	41.40	kJ/mol	307.50	NIST Webbook
rfi	1.40490		298.15	Volumetric, Viscometric, Ultrasonic, and Refractive Index Properties of Liquid Mixtures of Benzene with Industrially Important Monomers at Different Temperatures

rfi	1.40320		303.15	Volumetric, Viscometric, Ultrasonic, and Refractive Index Properties of Liquid Mixtures of Benzene with Industrially Important Monomers at Different Temperatures
rfi	1.40140		308.15	Volumetric, Viscometric, Ultrasonic, and Refractive Index Properties of Liquid Mixtures of Benzene with Industrially Important Monomers at Different Temperatures
rfi	1.39990		313.15	Volumetric, Viscometric, Ultrasonic, and Refractive Index Properties of Liquid Mixtures of Benzene with Industrially Important Monomers at Different Temperatures
rhol	936.25	kg/m3	280.65	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	916.12	kg/m3	298.15	Volumetric Properties of 3-Methylbutyl Ethanoate with Ethyl Acrylate, Butyl Acrylate, Methyl Methacrylate, and Styrene at 25 C
rhol	915.95	kg/m3	298.15	Densities and volumetric properties of binary mixtures of N,N-dimethylformamide/N,N-dimethylacetamide with some alkyl acrylates at temperatures from 288.15 K to 318.15 K

rhol	939.09	kg/m3	278.15	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	921.00	kg/m3	293.00	KDB
rhol	933.39	kg/m3	283.15	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	930.52	kg/m3	285.65	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	927.65	kg/m3	288.15	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	924.78	kg/m3	290.65	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	921.90	kg/m3	293.15	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	919.01	kg/m3	295.65	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	916.12	kg/m3	298.15	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	913.22	kg/m3	300.65	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	910.32	kg/m3	303.15	Thermophysical Properties of Three Compounds from the Acrylate Family

rhol	907.41	kg/m3	305.65	Thermophysical Properties of Three Compounds from the Acrylate Family	
rhol	904.49	kg/m3	308.15	Thermophysical Properties of Three Compounds from the Acrylate Family	
rhol	901.56	kg/m3	310.65	Thermophysical Properties of Three Compounds from the Acrylate Family	
rhol	898.63	kg/m3	313.15	Thermophysical Properties of Three Compounds from the Acrylate Family	
rhol	895.68	kg/m3	315.65	Thermophysical Properties of Three Compounds from the Acrylate Family	
rhol	892.73	kg/m3	318.15	Thermophysical Properties of Three Compounds from the Acrylate Family	
rhol	889.77	kg/m3	320.65	Thermophysical Properties of Three Compounds from the Acrylate Family	
rhol	886.80	kg/m3	323.15	Thermophysical Properties of Three Compounds from the Acrylate Family	
rhol	883.82	kg/m3	325.65	Thermophysical Properties of Three Compounds from the Acrylate Family	
rhol	880.83	kg/m3	328.15	Thermophysical Properties of Three Compounds from the Acrylate Family	

rhol	877.83	kg/m3	330.65	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	874.83	kg/m3	333.15	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	871.81	kg/m3	335.65	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	868.78	kg/m3	338.15	Thermophysical Properties of Three Compounds from the Acrylate Family

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46709e+01
Coeff. B	-3.28201e+03
Coeff. C	-4.65160e+01
Temperature range (K), min.	274.70
Temperature range (K), max.	397.18

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.87203e+01
Coeff. B	-7.84512e+03
Coeff. C	-1.25776e+01
Coeff. D	1.02128e-05
Temperature range (K), min.	201.95
Temperature range (K), max.	553.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C140885&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1169
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Volumetric, Viscometric, Ultrasonic, and Refractive Index Properties of Liquid Mixtures of Benzene with Industrially Important Monomers at Different Temperatures:	https://www.doi.org/10.1007/s10765-009-0562-x
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Volumetric Properties of 3-Methylbutyl Ethanoate with Ethyl Acrylate, Butyl Acrylate, Methyl Methacrylate, and Styrene at 25 C:	https://www.doi.org/10.1007/s10765-005-5571-9
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Thermophysical Properties of Three Compounds from the Acrylate Family:	https://www.doi.org/10.1021/je301333b
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1169.mol
Densities and volumetric properties of (acetonitrile + alkyl acrylate monomer) binary mixtures at temperatures from 298.15 K to 318.15 K:	https://www.doi.org/10.1016/j.jct.2016.08.026
Temperature and concentration dependence of volumetric properties of (tetrahydrofuran + ethyl acrylate, or + ethyl acrylate, or + n-butyl acrylate, or + tert-butyl acrylate) binary mixtures:	https://www.doi.org/10.1016/j.jct.2016.10.042
Ultrasonic velocities, densities, and excess molar volumes of binary mixtures of N,N-dimethylformamide/N,N-dimethylacetamide with some alkyl acrylates at temperatures from 288.15 K to 318.15 K:	https://www.doi.org/10.1016/j.jct.2011.06.011
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Densities and volumetric properties of (tetrahydrofuran + methyl acrylate, or + ethyl acrylate, or + n-butyl acrylate, or + tert-butyl acrylate) binary mixtures:	https://www.doi.org/10.1016/j.jct.2012.10.015

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pvap:	Vapor pressure

rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility