2-Propenoic acid, methyl ester

Other names:	Acrylate de methyle Acrylic acid methyl ester Acrylsaeuremethylester CH2=CHCOOCH3 Curithane 103 METHOXYCARBONYLETHYLENE METHYL PROPENOATE Methyl 2-propenoate Methyl acrylate Methyl ester acrylic acid Methyl ester of 2-propenoic acid Methyl prop-2-enoate Methyl propenate Methyl-acrylat Methylacrylaat Methylester kyseliny akrylove Metilacrilato NSC 24146 UN 1919 acrylic acid, methyl ester propenoic acid, methyl ester
Inchi:	InChI=1S/C4H6O2/c1-3-4(5)6-2/h3H,1H2,2H3
InchiKey:	BAPJBEWLBFYGME-UHFFFAOYSA-N
Formula:	C4H6O2
SMILES:	C=CC(=O)OC
Mol. weight [g/mol]:	86.09
CAS:	96-33-3

Physical Properties

Property code	Value	Unit	Source
af	0.3500		KDB
affp	825.80	kJ/mol	NIST Webbook
basg	794.80	kJ/mol	NIST Webbook
chl	-2069.40 ± 0.67	kJ/mol	NIST Webbook
gf	-163.28	kJ/mol	Joback Method
hf	-333.00	kJ/mol	NIST Webbook

hfl	-362.20	kJ/mol	NIST Webbook
hfus	7.62	kJ/mol	Joback Method
hvap	29.20	kJ/mol	NIST Webbook
hvap	29.20	kJ/mol	NIST Webbook
ie	10.72	eV	NIST Webbook
ie	10.74	eV	NIST Webbook
ie	9.90	eV	NIST Webbook
log10ws	-0.22		Estimated Solubility Method
log10ws	-0.22		Aqueous Solubility Prediction Method
logp	0.345		Crippen Method
mcvol	70.360	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
nfpas	%!d(float64=2)		KDB
pc	4300.00	kPa	KDB
rinpol	568.00		NIST Webbook
rinpol	603.00		NIST Webbook
rinpol	569.00		NIST Webbook
rinpol	569.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	591.00		NIST Webbook
rinpol	595.00		NIST Webbook
rinpol	599.00		NIST Webbook
rinpol	566.00		NIST Webbook
rinpol	607.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	607.00		NIST Webbook
rinpol	598.00		NIST Webbook
rinpol	597.00		NIST Webbook
rinpol	602.00		NIST Webbook
rinpol	574.00		NIST Webbook
ripol	941.00		NIST Webbook
ripol	937.00		NIST Webbook
ripol	938.00		NIST Webbook
ripol	938.00		NIST Webbook
ripol	940.00		NIST Webbook
tb	353.70	K	NIST Webbook
tb	353.00	K	NIST Webbook
tb	354.10 ± 0.60	K	NIST Webbook
tb	353.00 ± 2.00	K	NIST Webbook
tb	353.50	K	KDB
tc	536.00	K	KDB

tf	197.50	K	NIST Webbook
tf	197.77	K	Aqueous Solubility Prediction Method
tf	196.70	K	KDB
tf	197.50 ± 0.20	K	NIST Webbook
vc	0.265	m3/kmol	KDB
zc	0.2556890		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	116.32	J/mol×K	363.89	Joback Method
cpg	128.49	J/mol×K	424.95	Joback Method
cpg	134.29	J/mol×K	455.47	Joback Method
cpg	139.91	J/mol×K	486.00	Joback Method
cpg	145.34	J/mol×K	516.53	Joback Method
cpg	150.58	J/mol×K	547.06	Joback Method
cpg	122.50	J/mol×K	394.42	Joback Method
cpl	133.40	J/mol×K	297.00	NIST Webbook
cpl	161.50	J/mol×K	298.15	NIST Webbook
cpl	172.30	J/mol×K	298.15	NIST Webbook
dvisc	0.0021165	Pa×s	205.24	Joback Method
dvisc	0.0004102	Pa×s	311.01	Joback Method
dvisc	0.0002583	Pa×s	363.89	Joback Method
dvisc	0.0003197	Pa×s	337.45	Joback Method
dvisc	0.0005515	Pa×s	284.56	Joback Method
dvisc	0.0007877	Pa×s	258.12	Joback Method
dvisc	0.0012203	Pa×s	231.68	Joback Method
hfust	9.73	kJ/mol	197.50	NIST Webbook
hfust	9.73	kJ/mol	197.50	NIST Webbook
hfust	9.73	kJ/mol	197.50	NIST Webbook
hvapt	38.00	kJ/mol	291.00	NIST Webbook
hvapt	28.80	kJ/mol	318.00	NIST Webbook
hvapt	34.20	kJ/mol	335.00	NIST Webbook

rfi	1.39540		308.15	Volumetric, Viscometric, Ultrasonic, and Refractive Index Properties of Liquid Mixtures of Benzene with Industrially Important Monomers at Different Temperatures	
rfi	1.39790		303.15	Volumetric, Viscometric, Ultrasonic, and Refractive Index Properties of Liquid Mixtures of Benzene with Industrially Important Monomers at Different Temperatures	
rfi	1.40000		298.15	Volumetric, Viscometric, Ultrasonic, and Refractive Index Properties of Liquid Mixtures of Benzene with Industrially Important Monomers at Different Temperatures	
rfi	1.39440		313.15	Volumetric, Viscometric, Ultrasonic, and Refractive Index Properties of Liquid Mixtures of Benzene with Industrially Important Monomers at Different Temperatures	
rhol	958.37	kg/m3	290.65	Thermophysical Properties of Three Compounds from the Acrylate Family	
rhol	927.41	kg/m3	315.65	Thermophysical Properties of Three Compounds from the Acrylate Family	

rhol	924.25	kg/m3	318.15	Thermophysical Properties of Three Compounds from the Acrylate Family	
rhol	921.09	kg/m3	320.65	Thermophysical Properties of Three Compounds from the Acrylate Family	
rhol	933.68	kg/m3	310.65	Thermophysical Properties of Three Compounds from the Acrylate Family	
rhol	914.73	kg/m3	325.65	Thermophysical Properties of Three Compounds from the Acrylate Family	
rhol	911.53	kg/m3	328.15	Thermophysical Properties of Three Compounds from the Acrylate Family	
rhol	908.31	kg/m3	330.65	Thermophysical Properties of Three Compounds from the Acrylate Family	
rhol	905.09	kg/m3	333.15	Thermophysical Properties of Three Compounds from the Acrylate Family	
rhol	901.85	kg/m3	335.65	Thermophysical Properties of Three Compounds from the Acrylate Family	
rhol	898.59	kg/m3	338.15	Thermophysical Properties of Three Compounds from the Acrylate Family	
rhol	955.98	kg/m3	293.00	KDB	

rhol	947.56	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	949.17	kg/m3	298.15	Self-aggregation of liquids from biomass in aqueous solution
rhol	973.52	kg/m3	278.15	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	970.51	kg/m3	280.65	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	967.49	kg/m3	283.15	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	964.46	kg/m3	285.65	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	936.80	kg/m3	308.15	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	939.91	kg/m3	305.65	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	943.00	kg/m3	303.15	Thermophysical Properties of Three Compounds from the Acrylate Family

rhol	961.42	kg/m3	288.15	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	946.10	kg/m3	300.65	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	949.17	kg/m3	298.15	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	952.25	kg/m3	295.65	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	955.31	kg/m3	293.15	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	930.55	kg/m3	313.15	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	917.91	kg/m3	323.15	Thermophysical Properties of Three Compounds from the Acrylate Family
sfust	49.26	J/mol×K	197.50	NIST Webbook
speedsl	1095.70	m/s	318.15	Ultrasonic study of molecular interactions in binary mixtures of methyl acrylate with 1-alkanols (C4 to C10) at temperatures from (288.15 to 318.15) K

speedsl	1139.10	m/s	308.15	Ultrasonic study of molecular interactions in binary mixtures of methyl acrylate with 1-alkanols (C4 to C10) at temperatures from (288.15 to 318.15) K
speedsl	1162.20	m/s	303.15	Ultrasonic study of molecular interactions in binary mixtures of methyl acrylate with 1-alkanols (C4 to C10) at temperatures from (288.15 to 318.15) K
speedsl	1183.60	m/s	298.15	Ultrasonic study of molecular interactions in binary mixtures of methyl acrylate with 1-alkanols (C4 to C10) at temperatures from (288.15 to 318.15) K
speedsl	1204.60	m/s	293.15	Ultrasonic study of molecular interactions in binary mixtures of methyl acrylate with 1-alkanols (C4 to C10) at temperatures from (288.15 to 318.15) K
speedsl	1226.60	m/s	288.15	Ultrasonic study of molecular interactions in binary mixtures of methyl acrylate with 1-alkanols (C4 to C10) at temperatures from (288.15 to 318.15) K
speedsl	1117.80	m/s	313.15	Ultrasonic study of molecular interactions in binary mixtures of methyl acrylate with 1-alkanols (C4 to C10) at temperatures from (288.15 to 318.15) K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47471e+01
Coeff. B	-3.18738e+03
Coeff. C	-3.90130e+01
Temperature range (K), min.	259.45
Temperature range (K), max.	376.82

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.86079e+01
Coeff. B	-6.30414e+03
Coeff. C	-7.99764e+00
Coeff. D	6.11250e-06
Temperature range (K), min.	196.32
Temperature range (K), max.	536.00

Sources

Ultrasonic study of molecular interactions in binary mixtures of methyl acrylate with 1-alkanols (C4 to C10) at temperatures from 298.15 K to 318.15 K:	https://www.doi.org/10.1016/j.jct.2012.11.027
Temperature and concentration dependence of volumetric properties of (1,4-dioxane + methyl 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
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Self-aggregation of liquids from biomass in aqueous solution:	https://www.doi.org/10.1016/j.jct.2013.06.020
Thermophysical Properties of Three Compounds from the Acrylate Family:	https://www.doi.org/10.1021/je301333b
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
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1166
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1166.mol
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96333&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Densities and volumetric properties of (acetonitrile + alkyl acrylate monomer) binary mixtures at temperatures from 293.15 K to 318.15 K:	https://www.doi.org/10.1016/j.jct.2016.08.026

Ultrasonic velocities, densities, and excess molar volumes of binary mixtures of N,N-dimethyl formamide with methyl acrylate, or ethyl acrylate, or butyl acrylate, or 2-ethyl hexyl acrylate at different temperatures
https://www.doi.org/10.1016/j.jct.2011.06.011

Densities and volumetric properties of binary mixtures of N,N-dimethyl formamide with methyl acrylate, or ethyl acrylate, or butyl acrylate, or 2-ethyl hexyl acrylate at different temperatures
https://www.doi.org/10.1016/j.jct.2012.10.015

Measurement and prediction of phase equilibria of ethylene + methyl acrylate + polyethylene-co-methyl acrylate) systems: Measurement and prediction of phase equilibria of ethylene + methyl acrylate + polyethylene-co-methyl acrylate) systems:
https://www.doi.org/10.1016/j.fluid.2018.03.005

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
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
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
sfust:	Entropy of fusion at a given temperature
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility