# 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: InChl=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	9.90	eV	NIST Webbook
ie	10.74	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
рс	4300.00	kPa	KDB
rinpol	569.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	607.00		NIST Webbook
rinpol	566.00		NIST Webbook
rinpol	599.00		
rinpol	607.00	NIST Webboo	
rinpol	591.00	NIST Webbook	
rinpol	597.00		NIST Webbook
rinpol	598.00		NIST Webbook
rinpol	602.00		NIST Webbook
rinpol	568.00		NIST Webbook
rinpol	574.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	569.00		NIST Webbook
rinpol	603.00		NIST Webbook
rinpol	595.00		NIST Webbook
ripol	938.00		NIST Webbook
ripol	941.00		NIST Webbook
ripol	940.00		NIST Webbook
ripol	938.00		NIST Webbook
ripol	937.00		NIST Webbook
tb	354.10 ± 0.60	K	NIST Webbook
tb	353.70	K	NIST Webbook
tb	353.00 ± 2.00	K	NIST Webbook
tb	353.00	K	NIST Webbook
tb	353.50	K	KDB
tc	536.00	K	KDB
	000.00		

tf	197.50	K	NIST Webbook
tf	197.50 ± 0.20	K	NIST Webbook
tf	197.77	К	Aqueous Solubility Prediction Method
tf	196.70	K	KDB
VC	0.265	m3/kmol	KDB
ZC	0.2556890		KDB

# **Temperature Dependent Properties**

Property code	Value	Unit	Temperature [K]	Source
cpg	128.49	J/mol×K	424.95	Joback Method
cpg	145.34	J/mol×K	516.53	Joback Method
cpg	139.91	J/mol×K	486.00	Joback Method
cpg	134.29	J/mol×K	455.47	Joback Method
cpg	122.50	J/mol×K	394.42	Joback Method
cpg	150.58	J/mol×K	547.06	Joback Method
cpg	116.32	J/mol×K	363.89	Joback Method
cpl	172.30	J/mol×K	298.15	NIST Webbook
cpl	133.40	J/mol×K	297.00	NIST Webbook
cpl	161.50	J/mol×K	298.15	NIST Webbook
dvisc	0.0005515	Paxs	284.56	Joback Method
dvisc	0.0004102	Paxs	311.01	Joback Method
dvisc	0.0003197	Paxs	337.45	Joback Method
dvisc	0.0021165	Paxs	205.24	Joback Method
dvisc	0.0007877	Paxs	258.12	Joback Method
dvisc	0.0012203	Paxs	231.68	Joback Method
dvisc	0.0002583	Paxs	363.89	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	1.40000		298.15	Volumetric, Viscometric, Viscometric, Ultrasonic, and Refractive Index Properties of Liquid Mixtures of Benzene with Industrially Important Monomers at Different Temperatures	
rfi	1.39540		308.15	Volumetric, Viscometric, 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, 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, Viscometric, Ultrasonic, and Refractive Index Properties of Liquid Mixtures of Benzene with Industrially Important Monomers at Different Temperatures	
rhol	921.09	kg/m3	320.65	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	905.09	kg/m3	333.15	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	914.73	kg/m3	325.65	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	917.91	kg/m3	323.15	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	927.41	kg/m3	315.65	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	933.68	kg/m3	310.65	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	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	958.37	kg/m3	290.65	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	967.49	kg/m3	283.15	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	973.52	kg/m3	278.15	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	949.17	kg/m3	298.15	Self-aggregation of liquids from biomass in aqueous solution
rhol	947.56	kg/m3	298.15	Densities and volumetric properties of binary mixtures of
			N,N-dimethyl	Iformamide/N,N-dimethylacetamide with some alkyl acrylates at temperatures from 288.15 K to 318.15 K
rhol	964.46	kg/m3	285.65	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	955.98	kg/m3	293.00	KDB
sfust	49.26	J/mol×K	197.50	NIST Webbook
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	
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	

# Correlations

Information Value

Property code	pvap
Equation	In(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

Densities and volumetric properties of https://www.doi.org/10.1016/j.jct.2012.10.015

Densities and volumetric properties of binary mixtures of NINAGAMI

https://www.doi.org/10.1016/j.fluid.2018.03.005

http://webbook.nist.gov/cgi/cbook.cgi?ID=C96333&Units=SI

Volumetric, Viscometric, Ultrasonic, and Refractive Index Properties of https://www.doi.org/10.1007/s10765-009-0562-x https://www.doi.org/10.1016/j.jct.2016.10.042 Lemberatzko en de Berentakon danasidenya na prolumation organisties of Britane na Maringler at meeting a crylate, or + http://pubs.acs.org/doi/abs/10.1021/ci990307l

ethyl acrylate, or + n-butyl acrylate, or + tentibulyl acrylate, or +

**Estimated Solubility Method:** http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl\_file/ci034243xsi20040112\_053635.txt

**KDB Vapor Pressure Data:** https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1166

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

The Yaws Handbook of Vapor https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Pressure: Self-aggregation of liquids from https://www.doi.org/10.1016/j.jct.2013.06.020

biomass in aqueous solution: KDB: https://www.cheric.org/files/research/kdb/mol/mol1166.mol

Joback Method: https://en.wikipedia.org/wiki/Joback\_method

#### Legend

af: Acentric Factoraffp: Proton affinitybasg: Gas basicity

**chl:** Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacitycpl: Liquid phase heat capacity

**dvisc:** Dynamic viscosity

gf: Standard Gibbs free energy of formationhf: 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/llogp: Octanol/Water partition coefficientmcvol: 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

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