2-Propenoic acid, butyl ester

Other names:	2-PROPENOIC ACID BUTYL ESTER
	ACRYLIC ACID BUTYL ESTER
	Acrylic acid, n-butyl ester
	BUTYL-2-PROPENOATE
	Butyl 2-propenoate
	Butyl acrylate
	Butylacrylate, inhibited
	Butylester kyseliny akrylove
	UN 2348
	acrylic acid, butyl ester
	butyl propenoate
	n-Butyl acrylate
	n-Butyl propenoate
	propenoic acid, butyl ester
Inchi:	InChI=1S/C7H12O2/c1-3-5-6-9-7(8)4-2/h4H,2-3,5-6H2,1H3
InchiKey:	CQEYYJKEWSMYFG-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	C=CC(=O)OCCCC
Mol. weight [g/mol]:	128.17
CAS:	141-32-2

Physical Properties

Property code	Value	Unit	Source
chl	-4046.96 ± 0.58	kJ/mol	NIST Webbook
gf	-138.02	kJ/mol	Joback Method
hf	-375.30 ± 0.80	kJ/mol	NIST Webbook
hf	-381.10	kJ/mol	NIST Webbook
hfl	-428.40	kJ/mol	NIST Webbook
hfl	-422.60 ± 0.70	kJ/mol	NIST Webbook
hfus	15.39	kJ/mol	Joback Method
hvap	47.31 ± 0.33	kJ/mol	NIST Webbook
hvap	47.30 ± 0.30	kJ/mol	NIST Webbook
hvap	47.30	kJ/mol	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.516		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB

nfpah	%!d(float64=2)		KDB
nfpas	%!d(float64=2)		KDB
pc	2840.00	kPa	Critical Point and Vapor Pressure Measurements for 17 Compounds by a Low Residence Time Flow Method
pc	4540.00 ± 350.00	kPa	NIST Webbook
rhoc	299.79 ± 15.38	kg/m3	NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	876.00		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	873.00		NIST Webbook
ripol	1178.00		NIST Webbook
ripol	1197.00		NIST Webbook
ripol	1197.00		NIST Webbook
ripol	1189.00		NIST Webbook
ripol	1175.00		NIST Webbook
ripol	1197.00		NIST Webbook
ripol	1169.00		NIST Webbook
ripol	1197.00		NIST Webbook
ripol	1189.00		NIST Webbook
tb	418.20	K	NIST Webbook
tb	420.20	K	NIST Webbook
tb	421.95	K	NIST Webbook
tc	644.00 ± 3.00	K	NIST Webbook
tf	209.50 ± 0.50	K	NIST Webbook
tf	209.15	K	NIST Webbook
tf	209.50	K	NIST Webbook
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.85	J/mol×K	432.53	Joback Method
cpg	233.32	J/mol×K	462.53	Joback Method
cpg	243.41	J/mol×K	492.54	Joback Method
cpg	253.12	J/mol×K	522.54	Joback Method
cpg	262.44	J/mol×K	552.54	Joback Method
cpg	271.40	J/mol×K	582.54	Joback Method
cpg	279.98	J/mol×K	612.55	Joback Method
cpl	251.00	J/mol×K	298.15	NIST Webbook
dvisc	0.0028577	Pa×s	239.05	Joback Method
dvisc	0.0015177	Pa×s	271.30	Joback Method
dvisc	0.0009221	Pa×s	303.54	Joback Method
dvisc	0.0003347	Pa×s	400.28	Joback Method
dvisc	0.0006165	Pa×s	335.79	Joback Method
dvisc	0.0004423	Pa×s	368.04	Joback Method
dvisc	0.0002641	Pa×s	432.53	Joback Method
hfust	17.31	kJ/mol	209.50	NIST Webbook
hfust	17.31	kJ/mol	209.50	NIST Webbook
hfust	17.31	kJ/mol	209.50	NIST Webbook
hvapt	42.80 ± 0.30	kJ/mol	368.50	NIST Webbook
hvapt	45.70 ± 0.30	kJ/mol	368.50	NIST Webbook
hvapt	40.00 ± 0.30	kJ/mol	368.50	NIST Webbook
hvapt	44.80	kJ/mol	346.50	NIST Webbook
rfi	1.40690		313.15	Volumetric, Viscometric, Ultrasonic, and Refractive Index Properties of Liquid Mixtures of Benzene with Industrially Important Monomers at Different Temperatures
rfi	1.40840		308.15	Volumetric, Viscometric, Ultrasonic, and Refractive Index Properties of Liquid Mixtures of Benzene with Industrially Important Monomers at Different Temperatures

rfi	1.41020		303.15	Volumetric, Viscometric, Ultrasonic, and Refractive Index Properties of Liquid Mixtures of Benzene with Industrially Important Monomers at Different Temperatures
rfi	1.41190		298.15	Volumetric, Viscometric, Ultrasonic, and Refractive Index Properties of Liquid Mixtures of Benzene with Industrially Important Monomers at Different Temperatures
rhol	901.56	kg/m3	290.65	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	899.07	kg/m3	293.15	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	896.59	kg/m3	295.65	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	894.10	kg/m3	298.15	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	891.61	kg/m3	300.65	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	904.04	kg/m3	288.15	Thermophysical Properties of Three Compounds from the Acrylate Family

rhol	886.61	kg/m3	305.65	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	884.11	kg/m3	308.15	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	881.61	kg/m3	310.65	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	879.10	kg/m3	313.15	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	876.58	kg/m3	315.65	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	874.07	kg/m3	318.15	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	871.55	kg/m3	320.65	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	869.02	kg/m3	323.15	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	866.49	kg/m3	325.65	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	863.95	kg/m3	328.15	Thermophysical Properties of Three Compounds from the Acrylate Family

rhol	861.41	kg/m3	330.65	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	858.86	kg/m3	333.15	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	856.31	kg/m3	335.65	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	853.75	kg/m3	338.15	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	893.95	kg/m3	298.15	Volumetric Properties of 3-Methylbutyl Ethanoate with Ethyl Acrylate, Butyl Acrylate, Methyl Methacrylate, and Styrene at 25 C
rhol	906.51	kg/m3	285.65	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	908.99	kg/m3	283.15	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	911.47	kg/m3	280.65	Thermophysical Properties of Three Compounds from the Acrylate Family
rhol	913.92	kg/m3	278.15	Thermophysical Properties of Three Compounds from the Acrylate Family

rhol	894.10	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	893.96	kg/m3	298.15	Densities and volumes of mixing of the ternary system toluene + butyl acrylate + methyl methacrylate and its binaries at 298.15 K
rhol	875.10	kg/m3	318.15	Densities and Volumetric Properties of Binary Mixtures of Butyl Acrylate with Benzene, Toluene, o-Xylene, m-Xylene, p-Xylene, and Mesitylene at Temperatures from 288.15 K to 318.15 K
rhol	879.85	kg/m3	313.15	Densities and Volumetric Properties of Binary Mixtures of Butyl Acrylate with Benzene, Toluene, o-Xylene, m-Xylene, p-Xylene, and Mesitylene at Temperatures from 288.15 K to 318.15 K
rhol	884.60	kg/m3	308.15	Densities and Volumetric Properties of Binary Mixtures of Butyl Acrylate with Benzene, Toluene, o-Xylene, m-Xylene, p-Xylene, and Mesitylene at Temperatures from 288.15 K to 318.15 K

rhol	889.35	kg/m3	303.15	Densities and Volumetric Properties of Binary Mixtures of Butyl Acrylate with Benzene, Toluene, o-Xylene, m-Xylene, p-Xylene, and Mesitylene at Temperatures from 288.15 K to 318.15 K
rhol	894.10	kg/m3	298.15	Densities and Volumetric Properties of Binary Mixtures of Butyl Acrylate with Benzene, Toluene, o-Xylene, m-Xylene, p-Xylene, and Mesitylene at Temperatures from 288.15 K to 318.15 K
rhol	898.85	kg/m3	293.15	Densities and Volumetric Properties of Binary Mixtures of Butyl Acrylate with Benzene, Toluene, o-Xylene, m-Xylene, p-Xylene, and Mesitylene at Temperatures from 288.15 K to 318.15 K
rhol	903.60	kg/m3	288.15	Densities and Volumetric Properties of Binary Mixtures of Butyl Acrylate with Benzene, Toluene, o-Xylene, m-Xylene, p-Xylene, and Mesitylene at Temperatures from 288.15 K to 318.15 K
rhol	889.11	kg/m3	303.15	Thermophysical Properties of Three Compounds from the Acrylate Family
sfust	82.61	J/mol×K	209.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57206e+01
Coeff. B	-3.99833e+03
Coeff. C	-5.80630e+01
Temperature range (K), min.	317.14
Temperature range (K), max.	442.18

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.67290e+01
Coeff. B	-7.34218e+03
Coeff. C	-7.50837e+00
Coeff. D	4.00837e-06
Temperature range (K), min.	208.55
Temperature range (K), max.	598.00

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Densities and volumes of mixing of the ternary system toluene + butyl acrylate + methyl methacrylate and its binaries at 298.15 K:	https://www.doi.org/10.1016/j.jct.2006.05.012
Densities and volumetric properties of binary mixtures of N,N-dimethylformamide/N,N-dimethylacetamide with methyl methacrylate and its binaries at 298.15 K:	https://www.doi.org/10.1016/j.jct.2012.10.015
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
NIST WebBook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C141322&Units=SI
Critical Point and Vapor Pressure Measurements for 17 Compounds by a Low-Residence-Time Flow Method:	https://www.doi.org/10.1021/je060269j
Ultrasonic velocities, densities, and excess molar volumes of binary mixtures of N,N-dimethylformamide with methyl acrylate, or ethyl acrylate, or butyl acrylate, or 2-ethyl hexyl acrylate at T = 308.15 K:	https://www.doi.org/10.1016/j.jct.2011.06.011
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1181
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
Densities and Volumetric Properties of Binary Mixtures of Butyl Acrylate with Benzene, Toluene, o-Xylene, m-Xylene, p-Xylene, and Mesitylene at Temperatures from 288.15 K to 318.15 K:	https://www.doi.org/10.1007/s10765-010-0768-y
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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1181.mol
Temperature and concentration dependence of 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.2016.10.042
Thermophysical Properties of Three Compounds from the Acrylate Family:	https://www.doi.org/10.1021/je301333b
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume