Butanoic acid, propyl ester

Other names:	Butyric acid, propyl ester
	N-PROPYL N-BUTYRATE
	PROPYL BUTANOATE
	PROPYL BUTYRATE
	PROPYL ESTER BUTYRIC ACID
	Propyl ester of butanoic acid
	Propyl n-butyrate
	Propylester kyseliny maselne
	n-Butyric acid n-propyl ester
	n-Propanol butyrate
	n-Propyl butyrate
	propyl bytanoate
Inchi:	InChI=1S/C7H14O2/c1-3-5-7(8)9-6-4-2/h3-6H2,1-2H3
InchiKey:	HUAZGNHGCJGYNP-UHFFFAOYSA-N
Formula:	C7H14O2
SMILES:	CCCOC(=O)CCC
Mol. weight [g/mol]:	130.18
CAS:	105-66-8

Physical Properties

Property code	Value	Unit	Source
chl	-4187.80	kJ/mol	NIST Webbook
dm	1.80	debye	KDB
gf	-225.86	kJ/mol	Joback Method
hf	-432.61	kJ/mol	Joback Method
hfus	16.67	kJ/mol	Joback Method
hvap	40.33	kJ/mol	Joback Method
log10ws	-1.92		Aqueous Solubility Prediction Method
logp	1.740		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	2710.00	kPa	KDB
pc	2720.00 ± 30.00	kPa	NIST Webbook
rinpol	135.60		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	891.00		NIST Webbook
rinpol	897.00		NIST Webbook

rinpol	881.50	NIST Webbook
rinpol	896.00	NIST Webbook
rinpol	885.00	NIST Webbook
rinpol	888.00	NIST Webbook
rinpol	880.00	NIST Webbook
rinpol	880.00	NIST Webbook
rinpol	875.00	NIST Webbook
rinpol	878.00	NIST Webbook
rinpol	884.00	NIST Webbook
rinpol	882.00	NIST Webbook
rinpol	884.00	NIST Webbook
rinpol	886.00	NIST Webbook
rinpol	879.00	NIST Webbook
rinpol	885.00	NIST Webbook
rinpol	885.00	NIST Webbook
rinpol	885.00	NIST Webbook
rinpol	885.00	NIST Webbook
rinpol	880.00	NIST Webbook
rinpol	892.00	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	875.00	NIST Webbook
rinpol	896.00	NIST Webbook
rinpol	916.00	NIST Webbook
rinpol	895.00	NIST Webbook
rinpol	865.00	NIST Webbook
rinpol	880.00	NIST Webbook
rinpol	895.00	NIST Webbook
rinpol	903.00	NIST Webbook
rinpol	897.00	NIST Webbook
rinpol	896.00	NIST Webbook
rinpol	898.00	NIST Webbook
rinpol	891.00	NIST Webbook
rinpol	898.00	NIST Webbook
rinpol	873.00	NIST Webbook
rinpol	896.00	NIST Webbook
rinpol	896.00	NIST Webbook
rinpol	893.00	NIST Webbook
rinpol	879.00	NIST Webbook
rinpol	881.00	NIST Webbook
rinpol	880.00	NIST Webbook
rinpol	881.00	NIST Webbook
rinpol	135.60	NIST Webbook
rinpol	877.00	NIST Webbook
rinpol	881.00	NIST Webbook

rinpol	884.00	NIST Webbook
rinpol	896.00	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	899.00	NIST Webbook
rinpol	899.00	NIST Webbook
rinpol	875.00	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	881.00	NIST Webbook
rinpol	891.00	NIST Webbook
rinpol	875.00	NIST Webbook
rinpol	887.00	NIST Webbook
rinpol	896.00	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	881.00	NIST Webbook
rinpol	880.00	NIST Webbook
rinpol	906.00	NIST Webbook
rinpol	912.00	NIST Webbook
rinpol	882.00	NIST Webbook
rinpol	881.00	NIST Webbook
rinpol	876.00	NIST Webbook
ripol	1137.00	NIST Webbook
ripol	1107.00	NIST Webbook
ripol	1110.00	NIST Webbook
ripol	1137.00	NIST Webbook
ripol	1107.00	NIST Webbook
ripol	1133.00	NIST Webbook
ripol	1120.00	NIST Webbook
ripol	1135.00	NIST Webbook
ripol	1126.00	NIST Webbook
ripol	1153.00	NIST Webbook
ripol	1156.00	NIST Webbook
ripol	1117.00	NIST Webbook
ripol	1110.00	NIST Webbook
ripol	1123.00	NIST Webbook
ripol	1133.00	NIST Webbook
ripol	1116.00	NIST Webbook
ripol	1098.00	NIST Webbook
ripol	1122.00	NIST Webbook
ripol	1127.00	NIST Webbook
ripol	1123.00	NIST Webbook
ripol	1110.00	NIST Webbook
ripol	1110.00	NIST Webbook
ripol	1110.00	NIST Webbook
ripol	1110.00	NIST Webbook

ripol	1136.00		NIST Webbook
tb	416.20	K	KDB
tc	593.70 ± 0.60	K	NIST Webbook
tc	600.00	K	KDB
tc	599.80 ± 5.00	K	NIST Webbook
tc	592.50 ± 0.60	K	NIST Webbook
tf	177.90	K	KDB
tf	177.95	K	Aqueous Solubility Prediction Method
tf	178.00 ± 0.50	K	NIST Webbook
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.48	J/mol×K	582.84	Joback Method
cpg	299.73	J/mol×K	612.24	Joback Method
cpg	238.65	J/mol×K	435.85	Joback Method
cpg	249.76	J/mol×K	465.25	Joback Method
cpg	260.50	J/mol×K	494.65	Joback Method
cpg	270.86	J/mol×K	524.04	Joback Method
cpg	280.85	J/mol×K	553.44	Joback Method
dvisc	0.0003401	Pa×s	403.34	Joback Method
dvisc	0.0002656	Pa×s	435.85	Joback Method
dvisc	0.0031909	Pa×s	240.81	Joback Method
dvisc	0.0016480	Pa×s	273.32	Joback Method
dvisc	0.0009795	Pa×s	305.82	Joback Method
dvisc	0.0006434	Pa×s	338.33	Joback Method
dvisc	0.0004549	Pa×s	370.84	Joback Method
hvapt	42.00	kJ/mol	385.50	NIST Webbook
hvapt	44.30	kJ/mol	343.50	NIST Webbook
hvapt	39.60	kJ/mol	410.00	NIST Webbook
rfi	1.39500		303.15	Correlation and Prediction of Excess Quantities and Vapor-Liquid Equilibria of Alkyl Esters + tert-Butyl Alcohol: Experimental Data for Propyl Esters + tert-Butyl Alcohol

rhol	867.90	kg/m3	298.15	Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) VII. HE m and VE m for 20 binary mixtures {xCu 1H2u 1CO2C3H7 + (1 x)a,x-ClCH2(CH2)v 2CH2Cl}, where u = 1 to 4, a = 1 and v = x = 2 to 6. An analysis of behavior using the COSMO-RS methodology
rhol	879.00	kg/m3	288.00	KDB

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	415.90	K	102.00	NIST Webbook
tbrp	312.40	K	1.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49207e+01
Coeff. B	-3.70105e+03
Coeff. C	-5.67560e+01
Temperature range (K), min.	309.68
Temperature range (K), max.	441.91

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.34865e+01
Coeff. B	-7.60502e+03
Coeff. C	-8.55915e+00

Coeff. D	5.25288e-06
Temperature range (K), min.	177.95
Temperature range (K), max.	594.00

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1088
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1088
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C105668&Units=SI
Correlation and Prediction of Excess Quantities and Vapor-Liquid Equilibria of Fatty Esters + tert-Butyl Alcohol:	https://www.doi.org/10.1021/je060003c
Grippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Experimental Data for Propyl Esters + tert-Butyl Alcohol:	
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) VII. HE m and VE m for 20 binary mixtures {xCu 1H2u 1CO2C3H7 + (1 x)a,x-ClCH2(CH2)v 2CH2Cl}, where u = 1 to 4, a = 1 and v = 1 = 2 to 6. An analysis of behavior using the COSMO-RS methodology:	https://www.doi.org/10.1016/j.jct.2008.10.007

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
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

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume