Propanoic acid, propyl ester

Other names:	NSC 72022
	PROPIONIC ACID N-PROPYL ESTER
	PROPYL PROPANOATE
	PROPYL PROPIONATE
	Propionic acid, propyl ester
	Propyl ester of propanoic acid
	Propylester kyseliny propionove
	methyl butyrate
	n-Propyl n-propanoate
	n-Propyl n-propionate
	n-Propyl propanoate
	n-Propyl propionate
Inchi:	InChI=1S/C6H12O2/c1-3-5-8-6(7)4-2/h3-5H2,1-2H3
InchiKey:	MCSINKKTEDDPNK-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	CCCOC(=O)CC
Mol. weight [g/mol]:	116.16
CAS:	106-36-5

Physical Properties

Property code	Value	Unit	Source
chl	-3545.00	kJ/mol	NIST Webbook
dm	1.80	debye	KDB
gf	-234.28	kJ/mol	Joback Method
hf	-411.97	kJ/mol	Joback Method
hfus	14.08	kJ/mol	Joback Method
hvap	35.60 ± 0.01	kJ/mol	NIST Webbook
hvap	43.48	kJ/mol	NIST Webbook
ie	9.96	eV	NIST Webbook
log10ws	-0.82		Aqueous Solubility Prediction Method
log10ws	-0.82		Estimated Solubility Method
logp	1.350		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3060.00 ± 30.00	kPa	NIST Webbook
pc	3020.00	kPa	KDB

rinpol	789.00	NIST Webbook
rinpol	792.40	NIST Webbook
rinpol	796.00	NIST Webbook
rinpol	793.00	NIST Webbook
rinpol	789.00	NIST Webbook
rinpol	810.00	NIST Webbook
rinpol	785.00	NIST Webbook
rinpol	792.60	NIST Webbook
rinpol	778.99	NIST Webbook
rinpol	800.00	NIST Webbook
rinpol	801.00	NIST Webbook
rinpol	785.00	NIST Webbook
rinpol	807.00	NIST Webbook
rinpol	794.00	NIST Webbook
rinpol	792.00	NIST Webbook
rinpol	792.00	NIST Webbook
rinpol	752.00	NIST Webbook
rinpol	759.00	NIST Webbook
rinpol	752.00	NIST Webbook
rinpol	789.00	NIST Webbook
rinpol	797.00	NIST Webbook
rinpol	792.00	NIST Webbook
rinpol	814.00	NIST Webbook
rinpol	795.00	NIST Webbook
rinpol	752.00	NIST Webbook
rinpol	796.00	NIST Webbook
rinpol	796.00	NIST Webbook
rinpol	789.00	NIST Webbook
rinpol	792.40	NIST Webbook
rinpol	814.00	NIST Webbook
rinpol	807.00	NIST Webbook
rinpol	809.00	NIST Webbook
rinpol	802.00	NIST Webbook
rinpol	811.00	NIST Webbook
rinpol	785.00	NIST Webbook
rinpol	751.00	NIST Webbook
rinpol	809.00	NIST Webbook
rinpol	807.00	NIST Webbook
rinpol	787.00	NIST Webbook
ripol	1065.00	NIST Webbook
ripol	1025.00	NIST Webbook
ripol	1056.00	NIST Webbook
ripol	1050.00	NIST Webbook
ripol	1065.00	NIST Webbook

ripol	1059.00		NIST Webbook
ripol	1023.00		NIST Webbook
ripol	1045.00		NIST Webbook
ripol	1032.00		NIST Webbook
ripol	1010.00		NIST Webbook
ripol	1043.00		NIST Webbook
ripol	1056.00		NIST Webbook
ripol	1080.00		NIST Webbook
ripol	1047.00		NIST Webbook
ripol	1050.00		NIST Webbook
ripol	1040.00		NIST Webbook
ripol	1042.00		NIST Webbook
ripol	1039.00		NIST Webbook
ripol	1064.00		NIST Webbook
ripol	1025.00		NIST Webbook
ripol	1008.00		NIST Webbook
tb	394.15 ± 1.00	K	NIST Webbook
tb	397.90 ± 1.00	K	NIST Webbook
tb	395.59 ± 2.00	K	NIST Webbook
tb	395.65 ± 1.00	K	NIST Webbook
tb	395.80 ± 1.50	K	NIST Webbook
tb	396.60 ± 0.30	K	NIST Webbook
tb	395.60	K	KDB
tb	395.51	K	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
tb	395.70	K	NIST Webbook
tb	395.60	K	NIST Webbook
tb	396.35 ± 0.50	K	NIST Webbook
tb	396.15 ± 0.50	K	NIST Webbook
tb	395.60 ± 1.00	K	NIST Webbook
tb	395.30 ± 0.50	K	NIST Webbook
tb	395.80 ± 0.30	K	NIST Webbook
tc	571.00 ± 1.00	K	NIST Webbook
tc	578.00	K	KDB
tc	578.00 ± 8.00	K	NIST Webbook
tc	563.70 ± 6.00	K	NIST Webbook
tc	578.00	K	NIST Webbook
tc	568.60 ± 0.60	K	NIST Webbook
tf	197.30 ± 0.30	K	NIST Webbook
tf	197.20	K	Aqueous Solubility Prediction Method
tf	197.20	K	KDB
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.87	J/mol×K	412.97	Joback Method
cpg	209.71	J/mol×K	442.57	Joback Method
cpg	219.25	J/mol×K	472.16	Joback Method
cpg	228.47	J/mol×K	501.76	Joback Method
cpg	237.38	J/mol×K	531.36	Joback Method
cpg	245.98	J/mol×K	560.96	Joback Method
cpg	254.27	J/mol×K	590.55	Joback Method
cpl	229.00	J/mol×K	298.38	NIST Webbook
cpl	226.65	J/mol×K	298.15	NIST Webbook
dvisc	0.0002729	Pa×s	412.97	Joback Method
dvisc	0.0016017	Pa×s	260.11	Joback Method
dvisc	0.0030279	Pa×s	229.54	Joback Method
dvisc	0.0006447	Pa×s	321.25	Joback Method
dvisc	0.0004605	Pa×s	351.83	Joback Method
dvisc	0.0003472	Pa×s	382.40	Joback Method
dvisc	0.0009687	Pa×s	290.68	Joback Method
hvapt	35.54	kJ/mol	395.60	NIST Webbook
hvapt	37.60	kJ/mol	392.00	NIST Webbook
hvapt	39.90	kJ/mol	365.00	NIST Webbook
hvapt	43.10	kJ/mol	327.50	NIST Webbook
hvapt	42.10 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	41.10 ± 0.10	kJ/mol	328.00	NIST Webbook
hvapt	38.80 ± 0.10	kJ/mol	358.00	NIST Webbook
hvapt	40.00 ± 0.10	kJ/mol	343.00	NIST Webbook
pvap	60.00	kPa	378.75	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	93.37	kPa	392.74	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	86.38	kPa	390.13	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane

pvap	77.90	kPa	386.81	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	70.32	kPa	383.56	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	60.83	kPa	379.07	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	51.21	kPa	373.82	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	47.90	kPa	371.88	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	40.92	kPa	367.30	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	33.58	kPa	361.75	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	101.30	kPa	395.51	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
rfi	1.38090		318.15	Thermodynamic properties of (an ester + and alkane). XVII. Experimental He and Ve values for (an alkyl propanoate + an alkane) at 318.15K

rfi	1.39060		298.15	Physical properties of (propyl propanoate + hexane + toluene) at 298.15 K
rfi	1.39050		298.15	Densities, Surface Tensions, and Refractive Indexes of Propyl Propanoate + Hexane + m-Xylene at 298.15 K
rfi	1.38820		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	881.00	kg/m3	293.00	KDB
rhol	875.61	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	875.53	kg/m3	298.10	Excess Molar Enthalpies of Propyl Propanoate + 1-Hexanol + Benzene at the Temperatures of 25 :C and 35 :C

rhol	881.62	kg/m3	298.15	Phase Equilibria for Reactive Distillation of Propyl Propanoate. Pure Component Property Data, Vapor-Liquid Equilibria, and Liquid-Liquid Equilibria
rhol	875.53	kg/m3	298.15	Surface Tension Deviations and Excess Molar Volumes on the Ternary System Propyl Propanoate + Hexane + p-Xylene at 298.15 K
srf	0.02	N/m	298.15	Experimental and theoretical surface tension deviations in the binary systems propyl propanoate + o-, m- and p-xylene at 298.15K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49902e+01
Coeff. B	-3.57685e+03
Coeff. C	-5.11410e+01
Temperature range (K), min.	294.42
Temperature range (K), max.	420.70

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.22076e+01
Coeff. B	-6.89668e+03
Coeff. C	-6.80611e+00
Coeff. D	3.05862e-06

Temperature range (K), min.	197.25
Temperature range (K), max.	578.00

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1078.mol
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Experimental determination and calculation of the critical curves for the binary systems of CO2 containing ketone, alkane, ester and alcohol, respectively:	https://www.doi.org/10.1016/j.fluid.2011.05.005
Surface Tension Deviations and Excess Molar Volumes on the Ternary System Propyl Propanoate + Hexane + p-Xylene at 298.15 K:	https://www.doi.org/10.1021/je900643r
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1078
Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) VII. HE m and VE m for 20 binary mixtures {xCu 1H2u 1CO2C3H7 + (1 x)aX-ClCH2(CH2)v 2CH2Cl}, where u = 1 to 4, a = 1 and v = 2 to 6 ... Analysis of behavior using the COSMO-RS methodology:	https://www.doi.org/10.1016/j.jct.2008.10.007
Phase Equilibria for Reactive Distillation of Propyl Propanoate. Pure Component Property Data, Vapor-Liquid Equilibria, and	https://www.doi.org/10.1021/je101302p
Liquid-liquid equilibrium of alcohol-ester systems with deep eutectic solvent on the base of choline chloride:	https://www.doi.org/10.1016/j.jct.2018.11.019
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Physical properties of (propyl propanoate + hexane + toluene) at 298.15 K:	https://www.doi.org/10.1016/j.jct.2006.08.011
Densities, Surface Tensions, and Refractive Indexes of Propyl Propanoate + Hexane + m-Xylene at 298.15 K:	https://www.doi.org/10.1021/je0504111
Correlation and Prediction of Excess Quantities and Vapor-Liquid Equilibria of Alkyl Esters + tert-Butyl Alcohol: Experimental Data for Propyl Esters + tert-Butyl Alcohol:	https://www.doi.org/10.1021/je060003c
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane:	https://www.doi.org/10.1021/acs.jced.5b01058
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Liquid-liquid equilibrium for the quaternary system propionic acid + n-propanol + n-propyl propionate + water at 293.15, 313.15 and 333.15 K:	https://www.doi.org/10.1016/j.fluid.2016.05.033
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106365&Units=SI
Experimental and theoretical surface tension deviations in the binary systems propyl propanoate + o-, m- and p-xylene at 298.15K:	https://www.doi.org/10.1016/j.fluid.2004.12.009
Thermodynamic properties of (an ester + and alkane). XVII. Experimental He and Ve values for (an alkyl propanoate + an alkane) at 318.15K:	https://www.doi.org/10.1016/j.jct.2004.12.014
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Vapor-Liquid Equilibrium Data of (Carbon Dioxide + Methyl Propionate) and (Carbon Dioxide + Propyl Propionate) at Pressures from (1.00 to 12.00) MPa and Temperatures from (313.0 to 373.0) K:	https://www.doi.org/10.1021/je9001784
Excess Molar Enthalpies of Propyl Propanoate + 1-Hexanol + Benzene at the Temperatures of 25 :C and 35 :C:	https://www.doi.org/10.1021/je0201370

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
ie:	Ionization energy
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
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume