Propanal

Other names:	1-Propanal
	1-Propanone
	Aldehyde propionique
	C2H5CHO
	Methylacetaldehyde
	NCI-C61029
	NSC 6493
	Propaldehyde
	Propanalaldehyde
	Propanaldehyde
	Propional
	Propionaldehyde
	Propionic aldehyde
	Proprionaldehyde
	Propylaldehyde
	Propylic aldehyde
	UN 1275
	ethanecarbaldehyde
	ethylcarboxaldehyde
	n-Propanal
	n-Propionaldehyde
Inchi:	InChI=1S/C3H6O/c1-2-3-4/h3H,2H2,1H3
InchiKey:	NBBJYMSMWIIQGU-UHFFFAOYSA-N
Formula:	C3H6O
SMILES:	CCC=O
Mol. weight [g/mol]:	58.08
CAS:	123-38-6

Physical Properties

Property code	Value	Unit	Source
af	0.3130		KDB
affp	786.00	kJ/mol	NIST Webbook
basg	754.00	kJ/mol	NIST Webbook
chl	-1816.50 ± 0.75	kJ/mol	NIST Webbook
dm	2.52	debye	KDB
ea	9.99e-04 ± 8.70e-05	eV	NIST Webbook

gf	-130.50	kJ/mol	KDB
hf	-192.00	kJ/mol	NIST Webbook
hf	-188.70 ± 0.75	kJ/mol	NIST Webbook
hf	-192.20	kJ/mol	KDB
hf	-190.60 ± 0.88	kJ/mol	NIST Webbook
hf	-186.00 ± 1.50	kJ/mol	NIST Webbook
hfl	-221.50 ± 0.75	kJ/mol	NIST Webbook
hfl	-218.30 ± 0.63	kJ/mol	NIST Webbook
hfl	-215.70 ± 1.50	kJ/mol	NIST Webbook
hfl	-220.20 ± 0.96	kJ/mol	NIST Webbook
hfus	5.82	kJ/mol	Joback Method
hvap	29.50	kJ/mol	NIST Webbook
hvap	29.70	kJ/mol	NIST Webbook
hvap	29.60	kJ/mol	NIST Webbook
hvap	29.70 ± 0.40	kJ/mol	NIST Webbook
hvap	29.64 ± 0.07	kJ/mol	NIST Webbook
hvap	29.70 ± 0.40	kJ/mol	NIST Webbook
hvap	30.00	kJ/mol	NIST Webbook
hvap	29.60	kJ/mol	NIST Webbook
hvap	29.60	kJ/mol	NIST Webbook
hvap	30.00	kJ/mol	NIST Webbook
hvap	29.96	kJ/mol	NIST Webbook
ie	9.99	eV	NIST Webbook
ie	9.85	eV	NIST Webbook
ie	9.96	eV	NIST Webbook
ie	9.98 ± 0.01	eV	NIST Webbook
ie	9.97 ± 0.01	eV	NIST Webbook
ie	9.95 ± 0.01	eV	NIST Webbook
ie	9.96 ± 0.01	eV	NIST Webbook
ie	9.95	eV	NIST Webbook
ie	9.82 ± 0.14	eV	NIST Webbook
ie	9.96	eV	NIST Webbook
ie	9.96	eV	NIST Webbook
ie	9.94	eV	NIST Webbook
log10ws	0.58		Aqueous Solubility Prediction Method
log10ws	0.58		Estimated Solubility Method
logp	0.595		Crippen Method
mcvol	54.700	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
nfpas	%!d(float64=1)		KDB
pc	5270.00	kPa	KDB
pc	5270.00 ± 100.00	kPa	NIST Webbook

pc	6869.83	kPa	NIST Webbook
pc	6869.84 ± 202.60	kPa	NIST Webbook
pc	5260.00 ± 60.00	kPa	NIST Webbook
pc	5270.00 ± 100.00	kPa	NIST Webbook
rhoc	285.17 ± 5.23	kg/m3	NIST Webbook
rinpol	468.00		NIST Webbook
rinpol	506.00		NIST Webbook
rinpol	473.63		NIST Webbook
rinpol	473.10		NIST Webbook
rinpol	473.00		NIST Webbook
rinpol	456.00		NIST Webbook
rinpol	480.00		NIST Webbook
rinpol	451.00		NIST Webbook
rinpol	511.00		NIST Webbook
rinpol	464.00		NIST Webbook
rinpol	461.00		NIST Webbook
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rinpol	473.00		NIST Webbook
rinpol	498.00		NIST Webbook
rinpol	511.00		NIST Webbook
rinpol	450.00		NIST Webbook
rinpol	480.00		NIST Webbook
rinpol	452.00		NIST Webbook
rinpol	473.00		NIST Webbook
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rinpol	470.00		NIST Webbook
rinpol	451.00		NIST Webbook
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rinpol	437.00		NIST Webbook
rinpol	475.00		NIST Webbook
rinpol	470.00		NIST Webbook
rinpol	461.00		NIST Webbook
rinpol	437.00		NIST Webbook
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rinpol	456.00		NIST Webbook
rinpol	479.00		NIST Webbook
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rinpol	480.00		NIST Webbook

rinpol	473.00	NIST Webbook
rinpol	473.00	NIST Webbook
rinpol	473.00	NIST Webbook
rinpol	474.00	NIST Webbook
rinpol	473.04	NIST Webbook
rinpol	472.74	NIST Webbook
rinpol	473.10	NIST Webbook
rinpol	472.71	NIST Webbook
rinpol	473.30	NIST Webbook
rinpol	473.50	NIST Webbook
rinpol	473.70	NIST Webbook
rinpol	473.63	NIST Webbook
rinpol	455.00	NIST Webbook
rinpol	472.00	NIST Webbook
ripol	788.00	NIST Webbook
ripol	790.00	NIST Webbook
ripol	799.00	NIST Webbook
ripol	790.00	NIST Webbook
ripol	800.00	NIST Webbook
ripol	797.00	NIST Webbook
ripol	816.00	NIST Webbook
ripol	798.00	NIST Webbook
ripol	828.00	NIST Webbook
ripol	827.00	NIST Webbook
ripol	826.00	NIST Webbook
ripol	784.00	NIST Webbook
ripol	808.00	NIST Webbook
ripol	783.00	NIST Webbook
ripol	823.00	NIST Webbook
ripol	784.00	NIST Webbook
ripol	800.00	NIST Webbook
ripol	801.00	NIST Webbook
ripol	747.00	NIST Webbook
ripol	804.00	NIST Webbook
ripol	780.00	NIST Webbook
ripol	763.00	NIST Webbook
ripol	769.00	NIST Webbook
ripol	809.00	NIST Webbook
ripol	816.00	NIST Webbook
ripol	790.00	NIST Webbook
ripol	782.00	NIST Webbook
ripol	795.00	NIST Webbook
ripol	762.00	NIST Webbook
ripol	800.00	NIST Webbook

ripol	784.00		NIST Webbook
ripol	823.00		NIST Webbook
ripol	827.00		NIST Webbook
ripol	790.00		NIST Webbook
ripol	801.00		NIST Webbook
ripol	748.00		NIST Webbook
ripol	801.00		NIST Webbook
ripol	784.00		NIST Webbook
ripol	800.00		NIST Webbook
ripol	801.00		NIST Webbook
ripol	807.00		NIST Webbook
ripol	762.00		NIST Webbook
ripol	762.00		NIST Webbook
ripol	762.00		NIST Webbook
ripol	784.00		NIST Webbook
ripol	784.00		NIST Webbook
ripol	798.00		NIST Webbook
ripol	816.50		NIST Webbook
ripol	808.80		NIST Webbook
ripol	810.40		NIST Webbook
ripol	812.90		NIST Webbook
ripol	784.00		NIST Webbook
sg	304.40 ± 1.60	J/mol×K	NIST Webbook
sl	212.90	J/mol×K	NIST Webbook
tb	321.00 ± 0.10	K	NIST Webbook
tb	321.00	K	KDB
tb	321.20	K	Isobaric (vapor + liquid) equilibria of 1-ethyl-3-methylimidazolium ethylsulfate plus (propionaldehyde or valeraldehyde): Experimental data and prediction
tb	322.00	K	NIST Webbook
tb	321.17 ± 0.30	K	NIST Webbook
tb	321.17 ± 0.05	K	NIST Webbook
tb	321.18	K	Isobaric Vapor-Liquid Equilibria for Binary and Ternary Mixtures of Propanal, Propanol, and Propanoic Acid
tb	321.10	K	NIST Webbook
tb	321.15	K	NIST Webbook
tb	321.15 ± 3.00	K	NIST Webbook
tb	323.45 ± 2.00	K	NIST Webbook
tb	321.92 ± 1.00	K	NIST Webbook
tb	321.70 ± 2.00	K	NIST Webbook

tb	321.70 ± 2.00	K	NIST Webbook
tb	322.15 ± 1.00	K	NIST Webbook
tb	321.15 ± 2.00	K	NIST Webbook
tb	323.15 ± 2.00	K	NIST Webbook
tb	322.15 ± 2.00	K	NIST Webbook
tb	341.65	K	NIST Webbook
tb	321.40 ± 2.00	K	NIST Webbook
tb	322.15 ± 2.00	K	NIST Webbook
tb	341.15	K	NIST Webbook
tb	322.65 ± 2.00	K	NIST Webbook
tb	322.15 ± 1.00	K	NIST Webbook
tb	320.85 ± 2.00	K	NIST Webbook
tb	321.15 ± 2.00	K	NIST Webbook
tb	321.15 ± 0.50	K	NIST Webbook
tb	323.15 ± 2.00	K	NIST Webbook
tb	322.65 ± 1.00	K	NIST Webbook
tb	321.25 ± 0.50	K	NIST Webbook
tb	322.65 ± 2.00	K	NIST Webbook
tb	319.40 ± 0.40	K	NIST Webbook
tb	321.20 ± 0.30	K	NIST Webbook
tb	321.15 ± 0.30	K	NIST Webbook
tb	321.85 ± 0.50	K	NIST Webbook
tb	323.44 ± 0.10	K	NIST Webbook
tb	323.44 ± 0.10	K	NIST Webbook
tb	321.65 ± 1.00	K	NIST Webbook
tb	321.08 ± 0.50	K	NIST Webbook
tb	324.15 ± 3.00	K	NIST Webbook
tb	320.55 ± 0.50	K	NIST Webbook
tb	321.15 ± 0.50	K	NIST Webbook
tb	321.20 ± 0.50	K	NIST Webbook
tb	321.12 ± 0.20	K	NIST Webbook
tc	532.60 ± 2.00	K	NIST Webbook
tc	504.40 ± 1.20	K	NIST Webbook
tc	504.40	K	KDB
tc	509.10 ± 4.00	K	NIST Webbook
tc	504.40 ± 0.70	K	NIST Webbook
tc	496.20	K	NIST Webbook
tc	805.75	K	NIST Webbook
tf	193.00 ± 8.00	K	NIST Webbook
tf	170.20 ± 1.00	K	NIST Webbook
tf	193.00 ± 2.00	K	NIST Webbook
tf	193.00	K	KDB
tf	171.60 ± 0.60	K	NIST Webbook
tf	193.10 ± 2.00	K	NIST Webbook

tf	192.00 ± 5.00	K	NIST Webbook
tf	192.65	K	Aqueous Solubility Prediction Method
tf	171.00 ± 4.00	K	NIST Webbook
tf	193.15	K	NIST Webbook
tt	171.32 ± 0.05	K	NIST Webbook
tt	171.15 ± 0.10	K	NIST Webbook
tt	171.32 ± 0.01	K	NIST Webbook
vc	0.204	m3/kmol	KDB
zc	0.2563470		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	84.53	J/mol×K	325.04	NIST Webbook
cpg	88.39	J/mol×K	350.07	NIST Webbook
cpg	92.22	J/mol×K	374.50	NIST Webbook
cpl	159.10	J/mol×K	298.15	NIST Webbook
cpl	134.70	J/mol×K	298.00	NIST Webbook
dvisc	0.0003400	Pa×s	293.15	Studies on physicochemical behavior of binary mixtures containing propanal and Alkan-2-ol
dvisc	0.0003300	Pa×s	298.15	Studies on physicochemical behavior of binary mixtures containing propanal and Alkan-2-ol
dvisc	0.0003100	Pa×s	303.15	Studies on physicochemical behavior of binary mixtures containing propanal and Alkan-2-ol
dvisc	0.0003000	Pa×s	308.15	Studies on physicochemical behavior of binary mixtures containing propanal and Alkan-2-ol

dvisc	0.0002700	Pa×s	318.15	Studies on physicochemical behavior of binary mixtures containing propanal and Alkan-2-ol
dvisc	0.0002500	Pa×s	323.15	Studies on physicochemical behavior of binary mixtures containing propanal and Alkan-2-ol
dvisc	0.0002800	Pa×s	313.15	Studies on physicochemical behavior of binary mixtures containing propanal and Alkan-2-ol
hfust	8.59	kJ/mol	171.30	NIST Webbook
hfust	8.59	kJ/mol	171.30	NIST Webbook
hfust	8.59	kJ/mol	171.32	NIST Webbook
hvapt	30.30	kJ/mol	286.00	NIST Webbook
hvapt	28.32	kJ/mol	321.08	NIST Webbook
hvapt	30.30	kJ/mol	306.00	NIST Webbook
hvapt	28.31	kJ/mol	321.10	NIST Webbook
hvapt	31.50	kJ/mol	318.00	NIST Webbook
hvapt	30.50	kJ/mol	303.50	NIST Webbook
hvapt	28.30	kJ/mol	321.00	NIST Webbook
hvapt	29.40	kJ/mol	303.00	NIST Webbook
hvapt	28.28	kJ/mol	322.00	KDB
hvapt	31.90	kJ/mol	290.00	NIST Webbook
pvap	101.30	kPa	321.20	Isobaric (vapor + liquid) equilibria of 1-ethyl-3-methylimidazolium ethylsulfate plus (propionaldehyde or valeraldehyde): Experimental data and prediction
pvap	101.33	kPa	321.18	Isobaric Vapor-Liquid Equilibria for Binary and Ternary Mixtures of Propanal, Propanol, and Propanoic Acid

rfi	1.36340 ± 0.00010		298.15	Isobaric Vapor-Liquid Equilibria for Binary and Ternary Mixtures of Propanal, Propanol, and Propanoic Acid
rfi	1.36440		293.15	Liquid-liquid equilibria of water + solutes (acetic acid/ acetol/furfural/guaiacol/methanol/phenol/propanal) + solvents (isopropyl acetate/toluene) ternary systems for pyrolysis oil fractionation
rhol	797.21 ± 0.01	kg/m3	298.15	Isobaric Vapor-Liquid Equilibria for Binary and Ternary Mixtures of Propanal, Propanol, and Propanoic Acid
rhol	790.30	kg/m3	303.15	Studies on physicochemical behavior of binary mixtures containing propanal and Alkan-2-ol
rhol	784.50	kg/m3	308.15	Studies on physicochemical behavior of binary mixtures containing propanal and Alkan-2-ol
rhol	779.00	kg/m3	313.15	Studies on physicochemical behavior of binary mixtures containing propanal and Alkan-2-ol
rhol	796.20	kg/m3	298.15	Studies on physicochemical behavior of binary mixtures containing propanal and Alkan-2-ol
rhol	802.40	kg/m3	293.15	Studies on physicochemical behavior of binary mixtures containing propanal and Alkan-2-ol

rhol	776.53	kg/m3	313.15	Isobaric (vapor + liquid) equilibria of 1-ethyl-3-methylimidazolium ethylsulfate plus (propionaldehyde or valeraldehyde): Experimental data and prediction
rhol	782.55	kg/m3	308.16	Isobaric (vapor + liquid) equilibria of 1-ethyl-3-methylimidazolium ethylsulfate plus (propionaldehyde or valeraldehyde): Experimental data and prediction
rhol	788.72	kg/m3	303.15	Isobaric (vapor + liquid) equilibria of 1-ethyl-3-methylimidazolium ethylsulfate plus (propionaldehyde or valeraldehyde): Experimental data and prediction
rhol	794.85	kg/m3	298.15	Isobaric (vapor + liquid) equilibria of 1-ethyl-3-methylimidazolium ethylsulfate plus (propionaldehyde or valeraldehyde): Experimental data and prediction
rhol	794.85	kg/m3	298.15	Isobaric (vapor + liquid) equilibria of 1-ethyl-3-methylimidazolium ethylsulfate plus (propionaldehyde or valeraldehyde): Experimental data and prediction

rhol	801.06	kg/m3	293.15	Isobaric (vapor + liquid) equilibria of 1-ethyl-3-methylimidazolium ethylsulfate plus (propionaldehyde or valeraldehyde): Experimental data and prediction
rhol	807.26	kg/m3	288.14	Isobaric (vapor + liquid) equilibria of 1-ethyl-3-methylimidazolium ethylsulfate plus (propionaldehyde or valeraldehyde): Experimental data and prediction
rhol	797.00	kg/m3	293.00	KDB
rhol	773.50	kg/m3	318.15	Studies on physicochemical behavior of binary mixtures containing propanal and Alkan-2-ol
rhol	768.20	kg/m3	323.15	Studies on physicochemical behavior of binary mixtures containing propanal and Alkan-2-ol
srf	0.03	N/m	298.20	KDB

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C123386&Units=SI

Isobaric Vapor-Liquid Equilibria for Binary and Ternary Mixtures of Propanal, Propanol, and Propanoic Acid: https://www.doi.org/10.1021/je100912t

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Isobaric (vapor + liquid) equilibria of 1-ethyl-3-methylimidazolium ethylsulfate plus (propionaldehyde or valeraldehyde): Experimental data and prediction: https://www.doi.org/10.1016/j.jct.2011.01.008

KDB: https://www.cheric.org/files/research/kdb/mol/mol1233.mol

Studies on physicochemical behavior of binary mixtures containing propanal and Alkan-2-ol: https://www.doi.org/10.1016/j.jct.2017.07.004

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Liquid-liquid equilibria of water + solutes (acetic acid/ acetol/furfural/guaiacol/methanol/phenol/propanal) + solvents (isopropyl acetate/toluene) ternary systems for pyrolysis oil fractionation: https://www.doi.org/10.1016/j.fluid.2018.04.016

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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

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
dm:	Dipole Moment
dvisc:	Dynamic viscosity
ea:	Electron affinity
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
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sg:	Molar entropy at standard conditions
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

zc: Critical Compressibility