Propane, 1-nitro-

Other names:	1-NP
	1-Nitropan
	1-Nitropropane
	N-Nitropropane
	NiPar S-10
	n-C3H7NO2
Inchi:	InChI=1S/C3H7NO2/c1-2-3-4(5)6/h2-3H2,1H3
InchiKey:	JSZOAYXJRCEYSX-UHFFFAOYSA-N
Formula:	C3H7NO2
SMILES:	CCC[N+](=O)[O-]
Mol. weight [g/mol]:	89.09
CAS:	108-03-2

Physical Properties

Property code	Value	Unit	Source
af	0.3760		KDB
chl	-2013.40 ± 2.60	kJ/mol	NIST Webbook
chl	-2000.00	kJ/mol	NIST Webbook
chl	-2014.00 ± 0.40	kJ/mol	NIST Webbook
chl	-2012.10 ± 1.20	kJ/mol	NIST Webbook
gf	9.93	kJ/mol	Joback Method
hf	-116.01	kJ/mol	Joback Method
hfl	-168.80 ± 1.30	kJ/mol	NIST Webbook
hfl	-167.00 ± 0.40	kJ/mol	NIST Webbook
hfl	-167.60 ± 2.60	kJ/mol	NIST Webbook
hfus	14.89	kJ/mol	Joback Method
hvap	43.39 ± 0.42	kJ/mol	NIST Webbook
hvap	43.90	kJ/mol	NIST Webbook
ie	10.81 ± 0.03	eV	NIST Webbook
ie	10.78 ± 0.03	eV	NIST Webbook
ie	10.75 ± 0.01	eV	NIST Webbook
ie	10.95	eV	NIST Webbook
log10ws	-0.80		Estimated Solubility Method
log10ws	-0.80		Aqueous Solubility Prediction Method
logp	0.673		Crippen Method

mcvol	70.550	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=1)		KDB
nfpas	%!d(float64=3)		KDB
pc	4000.00	kPa	KDB
rinpol	715.00		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	723.00		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	677.00		NIST Webbook
rinpol	710.00		NIST Webbook
rinpol	707.00		NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	711.00		NIST Webbook
rinpol	711.00		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	709.00		NIST Webbook
rinpol	711.00		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	706.00		NIST Webbook
rinpol	711.00		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	707.00		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	667.00		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	708.43		NIST Webbook
rinpol	702.92		NIST Webbook
rinpol	707.16		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	662.00		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	661.90		NIST Webbook
rinpol	710.00		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	724.00		NIST Webbook

rinpol	678.00		NIST Webbook
rinpol	667.00		NIST Webbook
rinpol	709.97		NIST Webbook
rinpol	707.16		NIST Webbook
rinpol	706.13		NIST Webbook
rinpol	704.26		NIST Webbook
rinpol	703.52		NIST Webbook
rinpol	702.92		NIST Webbook
rinpol	702.42		NIST Webbook
rinpol	702.10		NIST Webbook
rinpol	711.18		NIST Webbook
rinpol	709.77		NIST Webbook
rinpol	708.43		NIST Webbook
rinpol	705.13		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	660.50		NIST Webbook
ripol	1248.40		NIST Webbook
ripol	1220.00		NIST Webbook
ripol	1251.00		NIST Webbook
ripol	1218.00		NIST Webbook
ripol	1279.00		NIST Webbook
ripol	1216.40		NIST Webbook
ripol	1241.40		NIST Webbook
ripol	1246.10		NIST Webbook
ripol	1237.80		NIST Webbook
ripol	1233.80		NIST Webbook
ripol	1230.40		NIST Webbook
ripol	1227.20		NIST Webbook
ripol	1251.60		NIST Webbook
ripol	1218.00		NIST Webbook
ripol	1220.00		NIST Webbook
tb	404.70	K	KDB
tc	606.00	K	KDB
tf	168.59 ± 0.05	K	NIST Webbook
tf	169.16 ± 0.06	K	NIST Webbook
tf	165.00	K	KDB
vc	0.285	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	133.52	J/mol×K	419.88	Joback Method
cpg	141.31	J/mol×K	454.80	Joback Method
cpg	148.72	J/mol×K	489.72	Joback Method
cpg	155.75	J/mol×K	524.64	Joback Method
cpg	162.43	J/mol×K	559.56	Joback Method
cpg	168.75	J/mol×K	594.48	Joback Method
cpg	174.74	J/mol×K	629.40	Joback Method
hvapt	42.60	kJ/mol	349.00	NIST Webbook
hvapt	40.60	kJ/mol	367.50	NIST Webbook
rhol	996.10	kg/m3	298.15	Speed of sound as a function of temperature and pressure for propane derivatives

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52908e+01
Coeff. B	-3.95030e+03
Coeff. C	-3.43730e+01
Temperature range (K), min.	297.67
Temperature range (K), max.	430.22

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.95825e+01
Coeff. B	-7.26354e+03
Coeff. C	-7.96077e+00
Coeff. D	4.74813e-06
Temperature range (K), min.	169.16
Temperature range (K), max.	605.00

Sources

High selective water/butan-1-ol separation on investigation of limiting activity coefficients with	https://www.doi.org/10.1016/j.fluid.2017.06.001
Thermodynamics and selectivity of separation based on activity coefficients at infinite dilution of	https://www.doi.org/10.1016/j.jct.2016.06.028
Thermodynamics of activity coefficients at infinite dilution for organic solutes and	https://www.doi.org/10.1016/j.jct.2013.09.007
Wikipedia: Joback method	https://en.wikipedia.org/wiki/Joback_method
Activity coefficients at infinite dilution for organic solutes and water in	https://www.doi.org/10.1016/j.jct.2015.05.014
Activity coefficients at infinite dilution and physicochemical properties for	https://www.doi.org/10.1016/j.jct.2015.02.024
Critical Assessment of CO2 Solubility in Volatile Solvents at 298.15 K:	https://www.doi.org/10.1021/je101161d
New ionic liquid [P4,4,4,4][NTf2] in bio-butanol extraction on investigation of limiting activity	https://www.doi.org/10.1016/j.fluid.2018.07.028
Activity coefficients measurements for organic solutes and water in the ionic liquid	https://www.doi.org/10.1016/j.jct.2016.08.008
Activity coefficients at infinite dilution and physicochemical properties for	https://www.doi.org/10.1016/j.jct.2012.08.016
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Thermodynamics and activity coefficients at infinite dilution for	https://www.doi.org/10.1016/j.jct.2014.04.024
Activity coefficients at infinite dilution for organic solutes, water and fuels in the	https://www.doi.org/10.1021/je4001894
Separation of binary mixtures based on limiting activity coefficients using	https://www.doi.org/10.1016/j.fluid.2017.12.029
Experimental and theoretical study of interaction between organic	https://www.doi.org/10.1016/j.fluid.2014.06.021
Activity coefficients at infinite dilution for organic solutes and water in the ionic liquid	https://www.doi.org/10.1016/j.jct.2016.07.017
Activity coefficients at infinite dilution for organic solutes and water in the ionic liquid	https://www.doi.org/10.1016/j.jct.2016.12.016
Physicochemical properties and activity coefficients at infinite dilution for organic solutes and water in the	https://www.doi.org/10.1016/j.jct.2012.09.033
Activity coefficients at infinite dilution and physicochemical properties for	https://www.doi.org/10.1016/j.jct.2011.11.021
Separation of binary mixtures based on limiting activity coefficients using	https://www.doi.org/10.1016/j.fluid.2015.05.022
Thermodynamic study of molecular interactions and separation	https://www.doi.org/10.1016/j.fluid.2018.02.014
Activity coefficients at infinite dilution and physicochemical properties for	https://www.doi.org/10.1021/je500050p
Partition Coefficients of Organic Compounds in New Imidazolium and	https://www.doi.org/10.1021/je9003178
Separation of binary mixtures containing hexane/hex-1-ene	https://www.doi.org/10.1016/j.jct.2017.03.004
Measurements of activity coefficients at infinite dilution for organic solutes in	https://www.doi.org/10.1016/j.jct.2012.03.005
Evaluation of the performance of 1-cyanopropan-1-aminium	https://www.doi.org/10.1021/je201129y
Activity coefficients at infinite dilution and physicochemical properties for	https://www.doi.org/10.1016/j.jct.2012.01.019
Partition Coefficients of Organic Compounds in Four New	https://www.doi.org/10.1021/je200637v
Activity Coefficients at Infinite Dilution for Organic Compounds Dissolved in	https://www.doi.org/10.1021/je300692s
Partition Coefficients of Organic Compounds in Propyl Sulfonate-Functionalized Ionic	https://www.doi.org/10.1021/je060033f
Activity coefficients at infinite dilution and physicochemical properties for	https://www.doi.org/10.1021/je800754w
Activity coefficients at infinite dilution and physicochemical properties for	https://www.doi.org/10.1016/j.jct.2013.01.007
Activity coefficients at infinite dilution and physicochemical properties for	https://www.doi.org/10.1016/j.jct.2013.08.030
Measurements of activity coefficients at infinite dilution of organic solutes in	https://www.doi.org/10.1016/j.jct.2011.11.025
Partition Coefficients of Organic Compounds in Ionic Liquid 1-hexyl-3-methylimidazolium	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Ammonium ionic liquids in extraction of bio-butan-1-ol from water phase	https://www.doi.org/10.1016/j.fluid.2018.09.024
Activity Coefficients at Infinite Dilution of Organic Solutes and Water in	https://www.doi.org/10.1021/acs.jced.5b00980
Tributylethylphosphonium Diethylphosphate Using Gas Liquid Chromatography: Thermodynamic	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1431
A 1-alkylcyanopyridinium-based ionic liquid in the separation processes:	https://www.doi.org/10.1016/j.jct.2016.01.017
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108032&Units=SI
Measurement of activity coefficients at infinite dilution in	https://www.doi.org/10.1016/j.jct.2007.01.004
Activity coefficients at infinite dilution and physicochemical properties for	https://www.doi.org/10.1016/j.jct.2012.05.017
Activity coefficients at infinite dilution of organic solutes in	https://www.doi.org/10.1016/j.jct.2015.02.023

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Experimental and theoretically study of interaction between organic compounds and tricyanomethanide based ionic liquids:	https://www.doi.org/10.1016/j.jct.2014.12.027
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid 1-(2-hydroxyethyl)-3-methylimidazolium trifluorotris(perfluoroethyl)phosphate:	https://www.doi.org/10.1016/j.jct.2013.05.008
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1431
Solution thermodynamics near the liquid liquid critical point I. First-order excess derivatives:	https://www.doi.org/10.1016/j.fluid.2007.05.017
Measurements of activity coefficients at infinite dilution for organic solutes and water in the ionic liquid 1-butyl-1-methylpyrrolidinium tricyanomethanide:	https://www.doi.org/10.1016/j.jct.2013.07.004
Activity Coefficients at Infinite Dilution of Organic Compounds in 1-Butyl-3-methylimidazolium Tetrafluoroborate Using Inverse Gas Chromatography:	https://www.doi.org/10.1021/je800658v
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid trihexyl-tetradecyl-phosphonium tricyanomethanide:	https://www.doi.org/10.1016/j.jct.2018.01.003
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Separation of water/butan-1-ol based on activity coefficients at infinite dilution in 1,3-didecyl-2-methylimidazolium dicyanamide ionic liquid:	https://www.doi.org/10.1016/j.jct.2017.10.003
The use of ionic liquids for separation of binary hydrocarbons mixtures based on gamma infinity data measurements:	https://www.doi.org/10.1016/j.jct.2018.07.024
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid 1-(2-methoxyethyl)-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)-amide:	https://www.doi.org/10.1016/j.jct.2012.03.015
Thermodynamics and activity coefficients at infinite dilution for organic solutes, water and diols in the ionic liquid N-hexylisoquinolinium thiocyanate, [HiQuin][SCN] using GLC:	https://www.doi.org/10.1016/j.fluid.2018.06.013
Measurements of activity coefficients at infinite dilution for organic solutes and water in the ionic liquid 1-butyl-1-methylpyrrolidinium dicyanamide:	https://www.doi.org/10.1016/j.jct.2013.02.004
Study of interaction between organic compounds and mono- or dicationic oxygenated ionic liquids using gas chromatography:	https://www.doi.org/10.1016/j.fluid.2014.11.020
Activity Coefficients at Infinite Dilution of Organic Compounds in Four New Imidazolium-Based Ionic Liquids:	https://www.doi.org/10.1021/je200195q
Activity coefficients at infinite dilution of organic solvents and water in 1-butyl-3-methylimidazolium dicyanamide. A literature review of hexane/hex-1-ene separation:	https://www.doi.org/10.1016/j.fluid.2016.02.004
Separation of binary mixtures hexane/hex-1-ene, cyclohexane/cyclohexene and ethylbenzene/styrene based on gamma infinity data measurements:	https://www.doi.org/10.1016/j.jct.2017.11.017
Study of Ether-, Alcohol-, or Cyano-Functionalized Ionic Liquids Using Inverse Gas Chromatography:	https://www.doi.org/10.1021/je900838a

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
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

rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume