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	-2012.10 ± 1.20	kJ/mol	NIST Webbook
chl	-2014.00 ± 0.40	kJ/mol	NIST Webbook
chl	-2000.00	kJ/mol	NIST Webbook
chl	-2013.40 ± 2.60	kJ/mol	NIST Webbook
gf	9.93	kJ/mol	Joback Method
hf	-116.01	kJ/mol	Joback Method
hfl	-167.00 ± 0.40	kJ/mol	NIST Webbook
hfl	-168.80 ± 1.30	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	10.75 ± 0.01	eV	NIST Webbook
ie	10.95	eV	NIST Webbook
ie	10.81 ± 0.03	eV	NIST Webbook
ie	10.78 ± 0.03	eV	NIST Webbook
log10ws	-0.80		Aqueous Solubility Prediction Method
log10ws	-0.80		Estimated Solubility 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	662.00		NIST Webbook
rinpol	705.13		NIST Webbook
rinpol	706.13		NIST Webbook
rinpol	707.16		NIST Webbook
rinpol	660.50		NIST Webbook
rinpol	709.97		NIST Webbook
rinpol	667.00		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	710.00		NIST Webbook
rinpol	661.90		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	704.26		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	667.00		NIST Webbook
rinpol	712.00		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	703.52		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	715.00		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	686.00		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	702.92		NIST Webbook
rinpol	702.92		NIST Webbook
rinpol	707.16		NIST Webbook
rinpol	724.00		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	708.43		NIST Webbook
rinpol	708.00		NIST Webbook
ripol	1246.10		NIST Webbook
ripol	1237.80		NIST Webbook
ripol	1241.40		NIST Webbook
ripol	1216.40		NIST Webbook
ripol	1279.00		NIST Webbook
ripol	1218.00		NIST Webbook
ripol	1251.00		NIST Webbook
ripol	1220.00		NIST Webbook
ripol	1230.40		NIST Webbook
ripol	1220.00		NIST Webbook
ripol	1233.80		NIST Webbook
ripol	1227.20		NIST Webbook
ripol	1251.60		NIST Webbook
ripol	1248.40		NIST Webbook
ripol	1218.00		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

Critical Assessment of CO2 Solubility in Volatile Solvents at 298.15 K:	https://www.doi.org/10.1021/je101161d
Separation of aliphatic from aromatic hydrocarbons and sulphur compounds from fuel based on measurements of 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 and physicochemical properties for organic solutes and water in the ionic liquid 4-(2-methoxyethyl)-4-methylmorpholinium bis(trifluoromethylsulfonyl)-amide:	https://www.doi.org/10.1016/j.jct.2011.11.021
Separation of water/butan-1-ol based on activity coefficients at infinite dilution in dicyanamide ionic liquid:	https://www.doi.org/10.1016/j.jct.2017.10.003
New ionic liquid [R4,4,4,4][NTf2] in bio-butanol extraction: an investigation of activity coefficients:	https://www.doi.org/10.1016/j.fluid.2018.07.028
Experimental and theoretical study of interaction between organic compounds and tricyanomethanide based ionic liquids:	https://www.doi.org/10.1016/j.jct.2014.12.027
Thermodynamics and limiting activity coefficients measurements for organic solutes and water in the ionic liquid 1-dodecyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide:	https://www.doi.org/10.1016/j.jct.2016.08.008
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
Infinite Dilution Activity Coefficients of Solutes Dissolved in Two	https://www.doi.org/10.1021/je500050p
Activity Coefficients at Infinite Dilution for Organic Solutes Dissolved in Three 1-Alkyl-1-methylpyrrolidinium Bis(trifluoromethylsulfonyl)imide Ionic Liquids Bearing Short Linear Alkyl Side Chains of Three to Five Carbons:	https://www.doi.org/10.1021/je4001894
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.2017.03.004
Separation of binary mixtures hexane/hex-1-ene, cyclohexane/cyclohexene and ethylbenzene/styrene based on limiting activity coefficients:	https://www.doi.org/10.1016/j.jct.2017.11.017
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid 4-(3-hydroxypropyl)-4-methylmorpholinium bis(trifluoromethylsulfonyl)-amide:	https://www.doi.org/10.1016/j.jct.2015.02.024
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
Ammonium ionic liquids in extraction of bio-butan-1-ol from water phase using activity coefficients at infinite dilution:	https://www.doi.org/10.1016/j.fluid.2018.09.024
High selective water/butan-1-ol separation on investigation of limiting activity coefficients with [P8,8,8,8][NTf2] ionic liquid:	https://www.doi.org/10.1016/j.fluid.2017.06.001
Thermodynamics and activity coefficients at infinite dilution for organic solutes and water in the ionic liquid 1-butyl-1-methylmorpholinium tricyanomethanide:	https://www.doi.org/10.1016/j.jct.2013.08.030
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
A 1-alkylcyanopyridinium-based ionic liquid in the separation processes:	https://www.doi.org/10.1016/j.jct.2016.01.017
Thermodynamics and activity coefficients at infinite dilution for organic solutes in the ionic liquid 1-butyl-1-methylpyrrolidinium dicyanamide:	https://www.doi.org/10.1016/j.fluid.2018.06.013
Activity coefficients at infinite dilution for organic solutes and water in 1-ethyl-1-methylpyrrolidinium lactate:	https://www.doi.org/10.1016/j.jct.2015.05.014
Activity coefficients at infinite dilution of organic solutes in methylphosphonate based ionic liquids using gas-liquid chromatography:	https://www.doi.org/10.1016/j.jct.2015.02.023
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid 1-(2-methoxyethyl)-1-methylpyrrolidinium trifluorotris(perfluoroethyl)phosphate:	https://www.doi.org/10.1016/j.jct.2013.01.007
Activity coefficients at infinite dilution, physicochemical and thermodynamic properties for organic solutes and water in the ionic liquid ethyl-dimethyl-(2-methoxyethyl)ammonium trifluorotris(perfluoroethyl)phosphate:	https://www.doi.org/10.1016/j.jct.2015.05.022
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid	https://www.doi.org/10.1016/j.jct.2018.01.003
Measurements of activity coefficients at infinite dilution in trihexyltetradecyl phosphonium tricyanomethanide:	https://www.doi.org/10.1016/j.jct.2007.01.004
Partition Coefficients of Organic Compounds in New Imidazolium and Tetralkylammonium Based Ionic Liquids Using Inverse Gas Chromatography:	https://www.doi.org/10.1021/je9003178
Activity Coefficients at Infinite Dilution of Organic Compounds in Four New Imidazolium-Based Ionic Liquids:	https://www.doi.org/10.1021/je200195q
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
Measurements of activity coefficients at infinite dilution for organic solutes and water in N-hexylisoquinolinium thiocyanate, [HiQuin][SCN] using GLC:	https://www.doi.org/10.1016/j.jct.2013.02.004
Activity Coefficients at Infinite Dilution of Organic Solutes and Water in Tributylethylphosphonium Diethylphosphate Using Gas-Liquid Chromatography: Thermodynamic Properties of Mixtures Containing Ionic Liquids:	https://www.doi.org/10.1021/acs.jced.5b00980
Study of Ether-, Alcohol-, or Cyano-Functionalized Ionic Liquids Using Inverse Gas Chromatography:	https://www.doi.org/10.1021/je900838a
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108032&Units=SI
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
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1431
Partition Coefficients of Organic Compounds in Four New Tetraalkylammonium Bis(trifluoromethylsulfonyl)imide Ionic Liquids Using Inverse Gas Chromatography:	https://www.doi.org/10.1021/je200637v
Physicochemical properties and activity coefficients at infinite dilution for organic solutes and water in a novel bicyclic guanidinium superbase-derived protic ionic liquid:	https://www.doi.org/10.1016/j.jct.2012.09.033
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid 4-(2-methoxyethyl)-4-methylmorpholinium trifluorotris(perfluoroethyl)phosphate:	https://www.doi.org/10.1016/j.jct.2012.05.017
Activity Coefficients at Infinite Dilution of Organic Compounds in Using Inverse Gas Chromatography:	https://www.doi.org/10.1021/je800754w
Thermodynamic Properties of Mixtures Containing Ionic Liquids: Activity Coefficients at Infinite Dilution of Organic Compounds in 1-Propyl Boronic Acid-3-Alkylimidazolium Bromide and 1-Propenyl-3-alkylimidazolium Bromide Using Inverse Gas Chromatography:	https://www.doi.org/10.1021/je060033f
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Experimental and theoretical study of interaction between organic compounds and 1-(4-sulfobutyl)-3-methylimidazolium based ionic liquids:	https://www.doi.org/10.1016/j.fluid.2014.06.021

The study of activity coefficients at infinite dilution for organic solutes and water in 1-butyl-4-methylpyridinium dicyanamide. [B4MPy][DCA] using GLC:	https://www.doi.org/10.1016/j.jct.2013.09.007
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1431
Separation of binary mixtures based on limiting activity coefficients data using GLC:	https://www.doi.org/10.1016/j.fluid.2017.12.029
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid 1-(2-hydroxyethyl)-3-methylimidazolium bis{(trifluoromethyl)sulfonyl}imide:	https://www.doi.org/10.1016/j.jct.2013.05.008
Measurements of activity coefficients at infinite dilution for organic solutes and water in the ionic liquid 1-(2-hydroxyethyl)-3-methylimidazolium tetracyanoborate:	https://www.doi.org/10.1016/j.jct.2012.03.005
Activity Coefficients at Infinite Dilution of Organic Compounds in Trihexyl(tetradecyl)phosphonium Bis(trifluoromethylsulfonyl)amide:	https://www.doi.org/10.1021/je800658v
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid 1-hexyl-3-methylimidazolium bis{(trifluoromethyl)sulfonyl}imide:	https://www.doi.org/10.1021/je201129y
Triggering fractionation ionic Liquids for Solution thermodynamics near the liquid liquid critical point I. First-order 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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Speed of sound as a function of temperature and pressure for propane derivatives:	https://www.doi.org/10.1016/j.jct.2016.12.016
Measurements of activity coefficients at infinite dilution for organic solutes and water in the ionic liquid 1-hexyl-3-methylimidazolium tetracyanoborate:	https://www.doi.org/10.1016/j.jct.2011.11.025
Thermodynamic study of molecular interaction selectivity in separation processes. Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid 1-(2-hydroxyethyl)-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)amide:	https://www.doi.org/10.1016/j.jct.2018.02.014
Activity coefficients at infinite dilution for organic solutes and water in the ionic liquid 1-(2-hydroxyethyl)-1-methylpiperidinium bis(trifluoromethylsulfonyl)amide:	https://www.doi.org/10.1016/j.jct.2012.01.019
Activity Coefficients at Infinite Dilution for Organic Compounds Dissolved in 1-(2-Hydroxyethyl)-1-methylpiperidinium Bis(trifluoromethylsulfonyl)amide:	https://www.doi.org/10.1021/je300692s
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid 1-(2-hydroxyethyl)-4-methylpyridinium bis(trifluoromethylsulfonyl)amide:	https://www.doi.org/10.1016/j.jct.2012.08.016
Activity coefficients at infinite dilution for organic solutes and water in the ionic liquid 1-ethyl-3-methylimidazolium ethylsulfate:	https://www.doi.org/10.1016/j.jct.2014.04.024
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Activity coefficients at infinite dilution for organic solutes, water and diols in the ionic liquid choline bis(trifluoromethylsulfonyl)imide:	https://www.doi.org/10.1016/j.jct.2016.06.028
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Thermodynamics and selectivity of separation based on activity coefficients at infinite dilution of various solutes in 1-allyl-3-methylimidazolium bis{(trifluoromethyl)sulfonyl}imide ionic liquid:	

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