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	-167.60 ± 2.60	kJ/mol	NIST Webbook
hfl	-168.80 ± 1.30	kJ/mol	NIST Webbook
hfl	-167.00 ± 0.40	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	10.78 ± 0.03	eV	NIST Webbook
ie	10.75 ± 0.01	eV	NIST Webbook
ie	10.81 ± 0.03	eV	NIST Webbook
ie	10.95	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	710.00		NIST Webbook
rinpol	707.16		NIST Webbook
rinpol	702.92		NIST Webbook
rinpol	708.43		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	707.00		NIST Webbook
rinpol	708.43		NIST Webbook
rinpol	709.77		NIST Webbook
rinpol	711.18		NIST Webbook
rinpol	702.10		NIST Webbook
rinpol	702.42		NIST Webbook
rinpol	702.92		NIST Webbook
rinpol	703.52		NIST Webbook
rinpol	704.26		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	724.00		NIST Webbook
rinpol	661.90		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	662.00		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	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	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	725.00		NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	686.00		NIST Webbook
ripol	1246.10		NIST Webbook
ripol	1220.00		NIST Webbook
ripol	1218.00		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	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	1248.40		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	168.75	J/mol×K	594.48	Joback Method
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	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

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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