

Propane, 2-nitro-

Other names:	2-NP
	2-Nitropropane
	Dimethylnitromethane
	Isonitropropane
	NSC 5369
	Nipar S-20
	Nipar S-20 solvent
	Nipar S-30 solvent
	Nitroisopropane
	Rcra waste number U171
	i-C3H7NO2
	sec-Nitropropane
	«beta»-Nitropropane
	Â«betaÂ»-Nitropropane
Inchi:	InChI=1S/C3H7NO2/c1-3(2)4(5)6/h3H,1-2H3
InchiKey:	FGLBSLMDCBOPQK-UHFFFAOYSA-N
Formula:	C3H7NO2
SMILES:	CC(C)[N+](=O)[O-]
Mol. weight [g/mol]:	89.09
CAS:	79-46-9

Physical Properties

Property code	Value	Unit	Source
af	0.3340		KDB
chl	-1997.60 ± 0.71	kJ/mol	NIST Webbook
chl	-2000.70 ± 3.60	kJ/mol	NIST Webbook
gf	7.49	kJ/mol	Joback Method
hf	-121.29	kJ/mol	Joback Method
hfl	-183.20 ± 0.71	kJ/mol	NIST Webbook
hfl	-180.30 ± 0.84	kJ/mol	NIST Webbook
hfus	11.36	kJ/mol	Joback Method
hvap	41.30 ± 0.42	kJ/mol	NIST Webbook
hvap	43.90	kJ/mol	NIST Webbook
ie	10.74 ± 0.03	eV	NIST Webbook
ie	10.71 ± 0.05	eV	NIST Webbook
ie	10.48	eV	NIST Webbook
ie	10.77 ± 0.01	eV	NIST Webbook

log10ws	-0.62		Estimated Solubility Method
log10ws	-0.62		Aqueous Solubility Prediction Method
logp	0.671		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	4150.00	kPa	KDB
rinpol	676.00		NIST Webbook
rinpol	676.00		NIST Webbook
rinpol	660.00		NIST Webbook
rinpol	685.00		NIST Webbook
rinpol	672.00		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	672.00		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	685.00		NIST Webbook
rinpol	631.00		NIST Webbook
ripol	1109.00		NIST Webbook
ripol	1109.00		NIST Webbook
ripol	1129.00		NIST Webbook
tb	393.50 ± 0.60	K	NIST Webbook
tb	393.40 ± 0.05	K	NIST Webbook
tb	393.30	K	KDB
tb	393.50	K	NIST Webbook
tc	597.00	K	KDB
tf	180.00	K	KDB
tf	180.72	K	Aqueous Solubility Prediction Method
tf	181.83 ± 0.05	K	NIST Webbook
vc	0.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.38	J/mol×K	491.01	Joback Method
cpg	141.71	J/mol×K	455.23	Joback Method
cpg	176.19	J/mol×K	634.16	Joback Method
cpg	170.04	J/mol×K	598.37	Joback Method

cpg	163.54	J/mol×K	562.59	Joback Method
cpg	156.65	J/mol×K	526.80	Joback Method
cpg	133.62	J/mol×K	419.44	Joback Method
hvapt	40.90	kJ/mol	339.00	NIST Webbook
hvapt	35.15	kJ/mol	393.30	KDB
pvap	3.34	kPa	304.20	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	2.57	kPa	299.20	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	3.34	kPa	304.10	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	1.90	kPa	294.30	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	4.30	kPa	309.10	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	5.61	kPa	314.10	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods

pvap	5.56	kPa	314.10	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	1.95	kPa	294.20	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	1.46	kPa	289.30	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	1.09	kPa	284.40	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	1.09	kPa	284.40	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.80	kPa	279.50	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.83	kPa	279.60	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods

pvap	0.60	kPa	274.80	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.60	kPa	274.80	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.61	kPa	274.70	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.52250e+01
Coeff. B	-3.84564e+03
Coeff. C	-3.09300e+01
Temperature range (K), min.	288.38
Temperature range (K), max.	418.85

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	6.10809e+01
Coeff. B	-6.61815e+03
Coeff. C	-6.74802e+00
Coeff. D	4.35069e-06
Temperature range (K), min.	181.83
Temperature range (K), max.	594.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
Aliphatic nitroalkanes: Evaluation of thermochemical data with Empirical Solubility Method and computational methods:	https://www.doi.org/10.1016/j.tca.2017.07.001
Supplemental Experimental and NIST Webbook:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt http://webbook.nist.gov/cgi/cbook.cgi?ID=C79469&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Critical Assessment of CO2 Solubility in Volatile Solvents at 298.15 K: KDB:	https://www.doi.org/10.1021/je101161d https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1432
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1432

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
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

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