

1,2,3-Propanetriol, trinitrate

Other names:	1,2,3-PROPANETRIOL TRINITRATE
	1,2,3-Propanetriol, 1,2,3-trinitrate
	1,2,3-Propanetriyl Nitrate
	Adesitrin
	Angibid
	Anginine
	Angiolingual
	Angorin
	Aquo-trinitrosan
	Blasting gelatin
	Blasting oil
	Cardamist
	Chitamite
	Corangil
	Cordipatch
	Corditrine
	Coro-nitro
	Deponit
	Epinitril
	GTN
	Gilucor nitro
	Glonoin
	Glonoine oil
	Glycerin trinitrate
	Glycerol(trinitrate de)
	Glycerol, nitric acid triester
	Glyceroltrinitraat
	Glyceryl nitrate
	Glyceryl trinitrate
	Klavikordal
	Lenitral
	Myocon
	Myoglycerin
	NG
	NK-843
	NTG
	Niglin
	Niglycon
	Niong
	Nitora

Nitric acid triester of glycerol

Nitrin

Nitrine

Nitrine-TDC

Nitro Mack

Nitro-Bid

Nitro-Dur

Nitro-PRN

Nitro-Span

Nitro-lent

Nitrocine

Nitroderm

Nitrodisc

Nitrofortin

Nitrogard

Nitroglicerina

Nitrogliceryna

Nitroglin

Nitroglycerin, spirits of

Nitroglycerine, spirit of

Nitroglycerol

Nitroglyn

Nitrol

Nitrolan

Nitrolande

Nitrolar

Nitroletten

Nitrolingual

Nitrolingual Spray

Nitrolowe

Nitromel

Nitromex

Nitronal

Nitronet

Nitrong

Nitrorectal

Nitroretard

Nitrosigma

Nitrostabilin

Nitrostat

Nitrozell retard

Nysconitrine

Percutol

Perglotal
Perlinganit
Propanetriol Trinitrate
RCRA Waste number P081
Reminitrol
S.N.G.
SK-106N
SNG
Solinitrina
Solution glyceryl trinitrate
Soup
Spirit of glonoin
Spirit of glyceryl trinitrate
Spirit of trinitroglycerin
Spirits of nitroglycerin
Susadrin
Suscard
Sustac
Sustonit
Sutonit
TNG
Temponitrin
Transderm-Nitro TTS
Transderm-nitro
Transiderm-nitro
Tridil
Trinalgon
Triniplas
Trinitrin
Trinitroglycerin
Trinitroglycerol
Trinitrol
Trinitrosan
Vasoglyn
glycerol trinitrate
nitroglycerin
nitroglycerine
propane-1,2,3-triyl trinitrate

Inchi: InChI=1S/C3H5N3O9/c7-4(8)13-1-3(15-6(11)12)2-14-5(9)10/h3H,1-2H2
InchiKey: SNIOPGDIGTZGOP-UHFFFAOYSA-N
Formula: C3H5N3O9
SMILES: O=[N+](O)OCC(CO[N+](=O)[O-])O[N+](=O)[O-]
Mol. weight [g/mol]: 227.09

Physical Properties

Property code	Value	Unit	Source
chl	-1525.90 ± 0.80	kJ/mol	NIST Webbook
chl	-1541.20	kJ/mol	NIST Webbook
chl	-1525.50 ± 3.80	kJ/mol	NIST Webbook
chl	-1523.00 ± 4.00	kJ/mol	NIST Webbook
chl	-1527.00	kJ/mol	NIST Webbook
chl	-1536.00	kJ/mol	NIST Webbook
chl	-1523.00	kJ/mol	NIST Webbook
hf	-279.10 ± 2.70	kJ/mol	NIST Webbook
hfl	-353.90	kJ/mol	NIST Webbook
hfl	-371.10 ± 1.70	kJ/mol	NIST Webbook
hfl	-370.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-372.00 ± 4.00	kJ/mol	NIST Webbook
hfl	-375.00	kJ/mol	NIST Webbook
hfus	37.65	kJ/mol	Joback Method
hvap	92.00 ± 2.10	kJ/mol	NIST Webbook
ie	11.42	eV	Cheméo Relay (1.0)
log10ws	-2.22		Estimated Solubility Method
log10ws	-2.22		Aqueous Solubility Prediction Method
logp	-1.020		Crippen Method
mcvol	123.000	ml/mol	McGowan Method
rinpol	1372.91		NIST Webbook
rinpol	1364.54		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1356.07		NIST Webbook
rinpol	1366.09		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1387.00		NIST Webbook
tb	478.34	K	Cheméo Relay (1.0)
tf	286.65	K	Aqueous Solubility Prediction Method
tf	286.15	K	KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.14	J/mol×K	790.38	Joback Method
cpg	349.38	J/mol×K	832.92	Joback Method
cpg	355.73	J/mol×K	875.46	Joback Method
cpg	361.15	J/mol×K	918.00	Joback Method
cpg	365.60	J/mol×K	960.54	Joback Method
cpg	369.05	J/mol×K	1003.08	Joback Method
cpg	371.45	J/mol×K	1045.62	Joback Method
hfust	21.87	kJ/mol	285.50	NIST Webbook
hvapt	58.60	kJ/mol	462.00	NIST Webbook
hvapt	104.50	kJ/mol	333.00	NIST Webbook
pvap	0.11	kPa	373.15	Kinetics and enthalpy of nitroglycerin evaporation from double base propellants by isothermal thermogravimetry
pvap	2.13	kPa	423.15	Kinetics and enthalpy of nitroglycerin evaporation from double base propellants by isothermal thermogravimetry
pvap	3.87e-03	kPa	333.15	Kinetics and enthalpy of nitroglycerin evaporation from double base propellants by isothermal thermogravimetry
pvap	9.81e-03	kPa	343.15	Kinetics and enthalpy of nitroglycerin evaporation from double base propellants by isothermal thermogravimetry
pvap	0.02	kPa	353.15	Kinetics and enthalpy of nitroglycerin evaporation from double base propellants by isothermal thermogravimetry

pvap	0.05	kPa	363.15	Kinetics and enthalpy of nitroglycerin evaporation from double base propellants by isothermal thermogravimetry
pvap	4.60e-04	kPa	313.15	Kinetics and enthalpy of nitroglycerin evaporation from double base propellants by isothermal thermogravimetry
pvap	0.21	kPa	383.15	Kinetics and enthalpy of nitroglycerin evaporation from double base propellants by isothermal thermogravimetry
pvap	0.40	kPa	393.15	Kinetics and enthalpy of nitroglycerin evaporation from double base propellants by isothermal thermogravimetry
pvap	0.72	kPa	403.15	Kinetics and enthalpy of nitroglycerin evaporation from double base propellants by isothermal thermogravimetry
pvap	1.26	kPa	413.15	Kinetics and enthalpy of nitroglycerin evaporation from double base propellants by isothermal thermogravimetry
pvap	1.40e-03	kPa	323.15	Kinetics and enthalpy of nitroglycerin evaporation from double base propellants by isothermal thermogravimetry

pvap	3.48	kPa	433.15	Kinetics and enthalpy of nitroglycerin evaporation from double base propellants by isothermal thermogravimetry
pvap	5.52	kPa	443.15	Kinetics and enthalpy of nitroglycerin evaporation from double base propellants by isothermal thermogravimetry
pvap	8.54	kPa	453.15	Kinetics and enthalpy of nitroglycerin evaporation from double base propellants by isothermal thermogravimetry
pvap	12.90	kPa	463.15	Kinetics and enthalpy of nitroglycerin evaporation from double base propellants by isothermal thermogravimetry
pvap	19.06	kPa	473.15	Kinetics and enthalpy of nitroglycerin evaporation from double base propellants by isothermal thermogravimetry
pvap	27.59	kPa	483.15	Kinetics and enthalpy of nitroglycerin evaporation from double base propellants by isothermal thermogravimetry
pvap	39.20	kPa	493.15	Kinetics and enthalpy of nitroglycerin evaporation from double base propellants by isothermal thermogravimetry

pvap	54.73	kPa	503.15	Kinetics and enthalpy of nitroglycerin evaporation from double base propellants by isothermal thermogravimetry
pvap	75.19	kPa	513.15	Kinetics and enthalpy of nitroglycerin evaporation from double base propellants by isothermal thermogravimetry
pvap	101.77	kPa	523.15	Kinetics and enthalpy of nitroglycerin evaporation from double base propellants by isothermal thermogravimetry
pvap	1.40e-04	kPa	303.15	Kinetics and enthalpy of nitroglycerin evaporation from double base propellants by isothermal thermogravimetry
pvap	7.00e-05	kPa	298.15	Kinetics and enthalpy of nitroglycerin evaporation from double base propellants by isothermal thermogravimetry

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.06057e+01
Coeff. B	-3.24887e+03
Coeff. C	-9.93120e+01
Temperature range (K), min.	414.18
Temperature range (K), max.	712.97

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Kinetics and enthalpy of nitroglycerin evaporation from double base propellants by isothermal thermogravimetry:	https://www.doi.org/10.1016/j.tca.2010.06.014
Estimated Solubility Method:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1426
NIST Webbook:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Joback Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55630&Units=SI
Cheméo Relay (1.0):	https://en.wikipedia.org/wiki/Joback_method
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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