

Nitroglycerin

Other names: 1,2,3-PROPANETRIOL TRINITRATE
1,2,3-Propanetriol, 1,2,3-trinitrate
1,2,3-Propanetriol, 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
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
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
 Perglottal
 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
 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
gf	-236.41	kJ/mol	Joback Method
hf	-279.10 ± 2.70	kJ/mol	NIST Webbook
hfl	-353.90	kJ/mol	NIST Webbook
hfl	-370.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-371.10 ± 1.70	kJ/mol	NIST Webbook
hfl	-375.00	kJ/mol	NIST Webbook
hfl	-372.00 ± 4.00	kJ/mol	NIST Webbook
hfus	37.65	kJ/mol	Joback Method
hvap	92.00 ± 2.10	kJ/mol	NIST Webbook
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
pc	4368.40	kPa	Joback Method
rinpol	1364.54		NIST Webbook
rinpol	1356.07		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1356.07		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1372.91		NIST Webbook
rinpol	1366.09		NIST Webbook
rinpol	1356.00		NIST Webbook
tb	790.38	K	Joback Method
tc	1045.62	K	Joback Method
tf	286.65	K	Aqueous Solubility Prediction Method
tf	286.15	K	KDB
vc	0.497	m ³ /kmol	Joback Method

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	104.50	kJ/mol	333.00	NIST Webbook
hvapt	58.60	kJ/mol	462.00	NIST Webbook
pvap	0.05	kPa	363.15	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	4.60e-04	kPa	313.15	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	3.87e-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	7.00e-05	kPa	298.15	Kinetics and enthalpy of nitroglycerin evaporation from double base propellants by isothermal thermogravimetry
pvap	0.11	kPa	373.15	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	2.13	kPa	423.15	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

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

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

Legend

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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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