Nonanoic acid

Other names:	1-Nonanoic acid
	1-Octanecarboxylic acid
	Cirrasol 185a
	Emery 1203
	Emfac 1202
	Hexacid C-9
	N-PELARGONIC ACID
	NSC 62787
	Nonoic acid
	Nonylic acid
	Pelargic acid
	Pelargon
	Pelargonic acid
	n-Nonanoic acid
	n-Nonoic acid
	n-Nonylic acid
Inchi:	InChI=1S/C9H18O2/c1-2-3-4-5-6-7-8-9(10)11/h2-8H2,1H3,(H,10,11)
InchiKey:	FBUKVWPVBMHYJY-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CCCCCCCCC(=O)O
Mol. weight [g/mol]:	158.24
CAS:	112-05-0

Physical Properties

Property code	Value	Unit	Source
chl	-5456.10 ± 0.90	kJ/mol	NIST Webbook
chl	-5452.25 ± 0.96	kJ/mol	NIST Webbook
gf	-240.84	kJ/mol	Joback Method
hf	-575.60 ± 1.00	kJ/mol	NIST Webbook
hf	-579.50 ± 1.00	kJ/mol	NIST Webbook
hf	-579.50 ± 1.00	kJ/mol	NIST Webbook
hfl	-661.91 ± 0.96	kJ/mol	NIST Webbook
hfl	-658.00 ± 0.90	kJ/mol	NIST Webbook
hfus	24.75	kJ/mol	Joback Method
hvap	82.40 ± 0.40	kJ/mol	NIST Webbook
hvap	82.40 ± 0.40	kJ/mol	NIST Webbook

log10ws	-2.75		Aqueous Solubility Prediction Method
logp	2.822		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2346.36 ± 90.00	kPa	NIST Webbook
pc	2350.00 ± 200.00	kPa	NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1290.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1281.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1288.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1303.00		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1278.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1272.10		NIST Webbook
rinpol	1268.00		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	1290.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	217.59		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1281.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1275.00		NIST Webbook

rinpol	1269.00	NIST Webbook
rinpol	1267.00	NIST Webbook
rinpol	1276.00	NIST Webbook
rinpol	1280.00	NIST Webbook
rinpol	1256.00	NIST Webbook
rinpol	1256.00	NIST Webbook
rinpol	1280.00	NIST Webbook
rinpol	1280.00	NIST Webbook
rinpol	1283.00	NIST Webbook
rinpol	1272.00	NIST Webbook
rinpol	1273.00	NIST Webbook
rinpol	1255.00	NIST Webbook
rinpol	1263.00	NIST Webbook
rinpol	1272.00	NIST Webbook
rinpol	1273.00	NIST Webbook
rinpol	1273.00	NIST Webbook
rinpol	1273.00	NIST Webbook
rinpol	1271.00	NIST Webbook
rinpol	1275.00	NIST Webbook
rinpol	1264.00	NIST Webbook
rinpol	1271.00	NIST Webbook
rinpol	1271.00	NIST Webbook
rinpol	1280.00	NIST Webbook
rinpol	1278.00	NIST Webbook
rinpol	1269.00	NIST Webbook
rinpol	1260.00	NIST Webbook
rinpol	1261.00	NIST Webbook
rinpol	1260.00	NIST Webbook
rinpol	1256.00	NIST Webbook
rinpol	1274.00	NIST Webbook
rinpol	1280.00	NIST Webbook
rinpol	1260.00	NIST Webbook
rinpol	1308.00	NIST Webbook
rinpol	1272.00	NIST Webbook
rinpol	1272.00	NIST Webbook
rinpol	1272.00	NIST Webbook
rinpol	1273.00	NIST Webbook
rinpol	1273.00	NIST Webbook
rinpol	1277.00	NIST Webbook
rinpol	1275.00	NIST Webbook
rinpol	1237.00	NIST Webbook
rinpol	1283.00	NIST Webbook
rinpol	1275.00	NIST Webbook
rinpol	1275.00	NIST Webbook

rinpol	1280.00	NIST Webbook
rinpol	1319.00	NIST Webbook
rinpol	1278.00	NIST Webbook
rinpol	1278.00	NIST Webbook
rinpol	1282.00	NIST Webbook
rinpol	1275.00	NIST Webbook
rinpol	1280.00	NIST Webbook
rinpol	1260.00	NIST Webbook
rinpol	1288.00	NIST Webbook
rinpol	1260.00	NIST Webbook
rinpol	1273.00	NIST Webbook
rinpol	1275.00	NIST Webbook
rinpol	1272.00	NIST Webbook
rinpol	1267.00	NIST Webbook
rinpol	1269.00	NIST Webbook
rinpol	1279.00	NIST Webbook
rinpol	1280.00	NIST Webbook
rinpol	1262.00	NIST Webbook
rinpol	1248.00	NIST Webbook
rinpol	1270.00	NIST Webbook
rinpol	1262.00	NIST Webbook
rinpol	1263.00	NIST Webbook
rinpol	1271.00	NIST Webbook
rinpol	1267.00	NIST Webbook
rinpol	1270.00	NIST Webbook
rinpol	1244.00	NIST Webbook
rinpol	1278.00	NIST Webbook
rinpol	1275.00	NIST Webbook
rinpol	1226.00	NIST Webbook
rinpol	1267.00	NIST Webbook
rinpol	1266.00	NIST Webbook
rinpol	1282.00	NIST Webbook
rinpol	1279.00	NIST Webbook
rinpol	1247.00	NIST Webbook
rinpol	1239.00	NIST Webbook
rinpol	1249.00	NIST Webbook
rinpol	1271.00	NIST Webbook
rinpol	1271.00	NIST Webbook
rinpol	1308.00	NIST Webbook
rinpol	1265.00	NIST Webbook
rinpol	1275.00	NIST Webbook
rinpol	1297.00	NIST Webbook
rinpol	1265.00	NIST Webbook
rinpol	1241.00	NIST Webbook

rinpol	1280.00	NIST Webbook
rinpol	1264.00	NIST Webbook
rinpol	1264.00	NIST Webbook
rinpol	1300.00	NIST Webbook
rinpol	1265.00	NIST Webbook
rinpol	1253.00	NIST Webbook
rinpol	1270.00	NIST Webbook
rinpol	1243.00	NIST Webbook
rinpol	1279.00	NIST Webbook
rinpol	1279.00	NIST Webbook
rinpol	1285.00	NIST Webbook
rinpol	1267.00	NIST Webbook
rinpol	1276.00	NIST Webbook
rinpol	217.59	NIST Webbook
rinpol	214.30	NIST Webbook
rinpol	1288.00	NIST Webbook
rinpol	1263.00	NIST Webbook
ripol	2178.00	NIST Webbook
ripol	2181.00	NIST Webbook
ripol	2178.00	NIST Webbook
ripol	2149.00	NIST Webbook
ripol	2179.00	NIST Webbook
ripol	2193.00	NIST Webbook
ripol	2174.00	NIST Webbook
ripol	2130.00	NIST Webbook
ripol	2158.00	NIST Webbook
ripol	2132.00	NIST Webbook
ripol	2138.00	NIST Webbook
ripol	2173.00	NIST Webbook
ripol	2192.00	NIST Webbook
ripol	2157.00	NIST Webbook
ripol	2150.00	NIST Webbook
ripol	2169.00	NIST Webbook
ripol	2182.00	NIST Webbook
ripol	2132.00	NIST Webbook
ripol	2188.00	NIST Webbook
ripol	2132.00	NIST Webbook
ripol	2169.00	NIST Webbook
ripol	2171.00	NIST Webbook
ripol	2174.00	NIST Webbook
ripol	2174.00	NIST Webbook
ripol	2180.00	NIST Webbook
ripol	2144.00	NIST Webbook
ripol	2159.00	NIST Webbook

ripol	2193.00	NIST Webbook
ripol	2127.00	NIST Webbook
ripol	2173.00	NIST Webbook
ripol	2162.00	NIST Webbook
ripol	2124.00	NIST Webbook
ripol	2179.00	NIST Webbook
ripol	2144.00	NIST Webbook
ripol	2202.00	NIST Webbook
ripol	2173.00	NIST Webbook
ripol	2180.00	NIST Webbook
ripol	2149.00	NIST Webbook
ripol	2174.00	NIST Webbook
ripol	2135.00	NIST Webbook
ripol	2124.00	NIST Webbook
ripol	2194.00	NIST Webbook
ripol	2161.00	NIST Webbook
ripol	2181.00	NIST Webbook
ripol	2211.00	NIST Webbook
ripol	2166.00	NIST Webbook
ripol	2178.00	NIST Webbook
ripol	2181.00	NIST Webbook
ripol	2164.00	NIST Webbook
ripol	2164.00	NIST Webbook
ripol	2176.00	NIST Webbook
ripol	2128.00	NIST Webbook
ripol	2157.00	NIST Webbook
ripol	2157.00	NIST Webbook
ripol	2177.00	NIST Webbook
ripol	2132.00	NIST Webbook
ripol	2158.00	NIST Webbook
ripol	2158.00	NIST Webbook
ripol	2164.00	NIST Webbook
ripol	2157.00	NIST Webbook
ripol	2147.00	NIST Webbook
ripol	2130.00	NIST Webbook
ripol	2145.00	NIST Webbook
ripol	2119.00	NIST Webbook
ripol	2174.00	NIST Webbook
ripol	2178.00	NIST Webbook
ripol	2152.00	NIST Webbook
ripol	2163.00	NIST Webbook
ripol	2173.00	NIST Webbook
ripol	2146.00	NIST Webbook
ripol	2181.00	NIST Webbook

ripol	2168.00	NIST Webbook
ripol	2168.00	NIST Webbook
ripol	2168.00	NIST Webbook
ripol	2153.00	NIST Webbook
ripol	2169.00	NIST Webbook
ripol	2170.00	NIST Webbook
ripol	2176.00	NIST Webbook
ripol	2180.00	NIST Webbook
ripol	2182.00	NIST Webbook
ripol	2198.00	NIST Webbook
ripol	2210.00	NIST Webbook
ripol	2176.00	NIST Webbook
ripol	2196.00	NIST Webbook
ripol	2211.00	NIST Webbook
ripol	2173.00	NIST Webbook
ripol	2165.00	NIST Webbook
ripol	2192.00	NIST Webbook
ripol	2192.00	NIST Webbook
ripol	2172.00	NIST Webbook
ripol	2173.00	NIST Webbook
ripol	2196.00	NIST Webbook
ripol	2155.00	NIST Webbook
ripol	2165.00	NIST Webbook
ripol	2149.00	NIST Webbook
ripol	2175.00	NIST Webbook
ripol	2167.00	NIST Webbook
ripol	2124.00	NIST Webbook
ripol	2153.00	NIST Webbook
ripol	2137.00	NIST Webbook
ripol	2130.00	NIST Webbook
ripol	2192.00	NIST Webbook
ripol	2192.00	NIST Webbook
ripol	2192.00	NIST Webbook
ripol	2192.00	NIST Webbook
ripol	2192.00	NIST Webbook
ripol	2165.00	NIST Webbook
ripol	2127.00	NIST Webbook
ripol	2180.00	NIST Webbook
ripol	2123.00	NIST Webbook
ripol	2127.00	NIST Webbook
ripol	2194.00	NIST Webbook
ripol	2131.00	NIST Webbook
ripol	2140.00	NIST Webbook
ripol	2200.00	NIST Webbook

ripol	2150.00		NIST Webbook
ripol	2192.00		NIST Webbook
ripol	2184.00		NIST Webbook
ripol	2168.00		NIST Webbook
ripol	2170.00		NIST Webbook
ripol	2157.00		NIST Webbook
ripol	2157.00		NIST Webbook
ripol	2190.00		NIST Webbook
ripol	2176.00		NIST Webbook
ripol	2138.00		NIST Webbook
ripol	2192.00		NIST Webbook
ripol	2165.00		NIST Webbook
ripol	2162.00		NIST Webbook
ripol	2186.00		NIST Webbook
ripol	2192.00		NIST Webbook
ripol	2173.00		NIST Webbook
ripol	2177.00		NIST Webbook
ripol	2192.00		NIST Webbook
ripol	2175.00		NIST Webbook
ripol	2138.00		NIST Webbook
ripol	2138.00		NIST Webbook
ripol	2192.00		NIST Webbook
ripol	2192.00		NIST Webbook
ripol	2124.00		NIST Webbook
ripol	2128.00		NIST Webbook
ripol	2192.00		NIST Webbook
ripol	2192.00		NIST Webbook
ripol	2192.00		NIST Webbook
ripol	2134.00		NIST Webbook
ripol	2173.00		NIST Webbook
ripol	2192.00		NIST Webbook
ripol	2192.00		NIST Webbook
ripol	2192.00		NIST Webbook
ripol	2192.00		NIST Webbook
ripol	2192.00		NIST Webbook
ripol	2150.00		NIST Webbook
ripol	2192.00		NIST Webbook
ripol	2176.00		NIST Webbook
tb	526.15 ± 3.00	K	NIST Webbook
tb	527.15 ± 3.00	K	NIST Webbook
tb	527.15 ± 1.50	K	NIST Webbook
tb	522.15 ± 5.00	K	NIST Webbook
tb	527.15 ± 2.00	K	NIST Webbook

tb	528.40 ± 3.00	K	NIST Webbook
tb	526.65 ± 3.00	K	NIST Webbook
tb	521.65 ± 4.00	K	NIST Webbook
tb	527.70 ± 3.00	K	NIST Webbook
tb	523.15 ± 3.00	K	NIST Webbook
tb	523.00 ± 5.00	K	NIST Webbook
tb	527.55 ± 1.00	K	NIST Webbook
tb	523.15 ± 3.00	K	NIST Webbook
tb	527.15 ± 2.00	K	NIST Webbook
tb	533.15 ± 6.00	K	NIST Webbook
tb	528.20	K	NIST Webbook
tc	712.00 ± 3.00	K	NIST Webbook
tc	709.58 ± 3.00	K	NIST Webbook
tf	284.58	K	Aqueous Solubility Prediction Method
tt	285.53 ± 0.02	K	NIST Webbook
vc	0.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.84	J/mol×K	635.29	Joback Method
cpg	366.91	J/mol×K	579.34	Joback Method
cpg	355.23	J/mol×K	551.37	Joback Method
cpg	399.10	J/mol×K	663.26	Joback Method
cpg	408.92	J/mol×K	691.24	Joback Method
cpg	418.31	J/mol×K	719.21	Joback Method
cpg	378.11	J/mol×K	607.32	Joback Method
cpl	362.37	J/mol×K	298.15	NIST Webbook
cpl	333.90	J/mol×K	304.00	NIST Webbook
dvisc	0.0134123	Pa×s	301.94	Joback Method
dvisc	0.0038351	Pa×s	343.51	Joback Method
dvisc	0.0014369	Pa×s	385.08	Joback Method
dvisc	0.0006519	Pa×s	426.65	Joback Method
dvisc	0.0003403	Pa×s	468.23	Joback Method
dvisc	0.0001975	Pa×s	509.80	Joback Method
dvisc	0.0001244	Pa×s	551.37	Joback Method
hfust	20.31	kJ/mol	285.50	NIST Webbook
hvapt	76.90	kJ/mol	454.50	NIST Webbook
hvapt	85.30 ± 2.00	kJ/mol	302.50	NIST Webbook
hvapt	64.20	kJ/mol	435.00	NIST Webbook

rhol	870.10	kg/m3	338.10	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	846.70	kg/m3	368.00	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	858.40	kg/m3	353.10	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	834.10	kg/m3	383.10	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	881.90	kg/m3	323.10	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	893.80	kg/m3	308.00	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	906.00	kg/m3	290.30	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	822.30	kg/m3	398.10	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	810.30	kg/m3	413.00	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K

rhol	798.00	kg/m3	427.90	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56017e+01
Coeff. B	-4.57898e+03
Coeff. C	-1.10247e+02
Temperature range (K), min.	409.25
Temperature range (K), max.	555.23

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.17697e+02
Coeff. B	-1.88791e+04
Coeff. C	-2.88174e+01
Coeff. D	1.18731e-05
Temperature range (K), min.	285.55
Temperature range (K), max.	703.00

Sources

Solubility of Nonanoic (Pelargonic) Acid in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je700465u
Solubility of Small-Chain Carboxylic Acids in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je100504h
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K:	https://www.doi.org/10.1021/acs.jced.5b00971
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C112050&Units=SI

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=943

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
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
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
tt:	Triple Point Temperature
vc:	Critical Volume