1-Nonene

Other names:	1-C9H18
	N-NON-1-ENE
	NONENE
	NONYLENE
	NSC 73961
	Non-1-ene
	Nonene-(1)
Inchi:	InChI=1S/C9H18/c1-3-5-7-9-8-6-4-2/h3H,1,4-9H2,2H3
InchiKey:	JRZJOMJEPLMPRA-UHFFFAOYSA-N
Formula:	C9H18
SMILES:	C=CCCCCCCC
Mol. weight [g/mol]:	126.24
CAS:	124-11-8

Physical Properties

Property code	Value	Unit	Source
af	0.4300		KDB
ap	311.150	K	KDB
gf	112.80	kJ/mol	KDB
hcg	5965.13	kJ/mol	KDB
hcn	5568.988	kJ/mol	KDB
hf	-103.60	kJ/mol	KDB
hfus	17.79	kJ/mol	Joback Method
hvap	44.70 ± 0.20	kJ/mol	NIST Webbook
hvap	45.50	kJ/mol	NIST Webbook
ie	9.42 ± 0.01	eV	NIST Webbook
log10ws	-5.05		Estimated Solubility Method
log10ws	-5.05		Aqueous Solubility Prediction Method
logp	3.533		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
pc	2340.00	kPa	KDB
rhoc	239.85	kg/m3	NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	888.70		NIST Webbook

rinpol	888.00	NIST Webbook
rinpol	888.00	NIST Webbook
rinpol	890.00	NIST Webbook
rinpol	889.00	NIST Webbook
rinpol	889.00	NIST Webbook
rinpol	883.00	NIST Webbook
rinpol	883.00	NIST Webbook
rinpol	883.40	NIST Webbook
rinpol	883.00	NIST Webbook
rinpol	881.00	NIST Webbook
rinpol	882.00	NIST Webbook
rinpol	883.00	NIST Webbook
rinpol	882.00	NIST Webbook
rinpol	889.50	NIST Webbook
rinpol	890.30	NIST Webbook
rinpol	882.70	NIST Webbook
rinpol	883.00	NIST Webbook
rinpol	889.00	NIST Webbook
rinpol	882.20	NIST Webbook
rinpol	887.00	NIST Webbook
rinpol	883.00	NIST Webbook
rinpol	890.00	NIST Webbook
rinpol	895.00	NIST Webbook
rinpol	887.00	NIST Webbook
rinpol	894.00	NIST Webbook
rinpol	890.00	NIST Webbook
rinpol	889.20	NIST Webbook
rinpol	882.00	NIST Webbook
rinpol	890.00	NIST Webbook
rinpol	893.00	NIST Webbook
rinpol	892.00	NIST Webbook
rinpol	888.90	NIST Webbook
rinpol	889.50	NIST Webbook
rinpol	890.20	NIST Webbook
rinpol	895.90	NIST Webbook
rinpol	896.00	NIST Webbook
rinpol	884.00	NIST Webbook
rinpol	888.90	NIST Webbook
rinpol	889.50	NIST Webbook
rinpol	890.20	NIST Webbook
rinpol	889.00	NIST Webbook
rinpol	888.00	NIST Webbook
rinpol	888.92	NIST Webbook
rinpol	888.92	NIST Webbook

rinpol	888.98	NIST Webbook
rinpol	891.78	NIST Webbook
rinpol	891.75	NIST Webbook
rinpol	891.84	NIST Webbook
rinpol	887.00	NIST Webbook
rinpol	892.00	NIST Webbook
rinpol	889.00	NIST Webbook
rinpol	883.00	NIST Webbook
rinpol	894.00	NIST Webbook
rinpol	889.00	NIST Webbook
rinpol	892.00	NIST Webbook
rinpol	889.00	NIST Webbook
rinpol	893.00	NIST Webbook
rinpol	895.00	NIST Webbook
rinpol	891.00	NIST Webbook
rinpol	892.00	NIST Webbook
rinpol	880.00	NIST Webbook
rinpol	886.00	NIST Webbook
rinpol	891.00	NIST Webbook
rinpol	886.00	NIST Webbook
rinpol	888.00	NIST Webbook
rinpol	886.00	NIST Webbook
rinpol	886.00	NIST Webbook
rinpol	888.80	NIST Webbook
rinpol	886.00	NIST Webbook
rinpol	890.00	NIST Webbook
rinpol	884.00	NIST Webbook
rinpol	899.00	NIST Webbook
rinpol	892.00	NIST Webbook
rinpol	888.00	NIST Webbook
rinpol	887.00	NIST Webbook
rinpol	889.00	NIST Webbook
rinpol	880.00	NIST Webbook
rinpol	889.00	NIST Webbook
rinpol	882.00	NIST Webbook
rinpol	891.00	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	888.00	NIST Webbook
rinpol	889.00	NIST Webbook
rinpol	889.00	NIST Webbook
rinpol	887.00	NIST Webbook
rinpol	896.00	NIST Webbook
rinpol	889.00	NIST Webbook
rinpol	884.00	NIST Webbook

rinpol	889.00		NIST Webbook
rinpol	886.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	885.20		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	889.00		NIST Webbook
rinpol	889.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	879.00		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	882.80		NIST Webbook
ripol	931.00		NIST Webbook
ripol	929.00		NIST Webbook
ripol	923.00		NIST Webbook
ripol	930.00		NIST Webbook
ripol	952.00		NIST Webbook
ripol	953.00		NIST Webbook
ripol	950.00		NIST Webbook
ripol	950.00		NIST Webbook
ripol	946.00		NIST Webbook
ripol	949.80		NIST Webbook
ripol	949.70		NIST Webbook
ripol	950.50		NIST Webbook
ripol	947.70		NIST Webbook
ripol	949.80		NIST Webbook
ripol	950.50		NIST Webbook
ripol	929.00		NIST Webbook
ripol	960.00		NIST Webbook
sl	392.54	J/mol×K	NIST Webbook
tb	420.00	K	KDB
tc	594.00	K	KDB
tc	594.00 ± 1.00	K	NIST Webbook
tf	191.33	K	Aqueous Solubility Prediction Method
tf	191.80	K	KDB
tt	191.60 ± 0.00	K	NIST Webbook
tt	191.91 ± 0.00	K	NIST Webbook
vc	0.526	m3/kmol	KDB
vc	0.526	m3/kmol	NIST Webbook
zc	0.2492170		KDB
zra	0.25		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.31	J/mol×K	402.00	Joback Method
cpg	270.92	J/mol×K	429.72	Joback Method
cpg	284.01	J/mol×K	457.43	Joback Method
cpg	296.58	J/mol×K	485.15	Joback Method
cpg	308.66	J/mol×K	512.86	Joback Method
cpg	320.25	J/mol×K	540.58	Joback Method
cpg	331.38	J/mol×K	568.30	Joback Method
cpl	270.36	J/mol×K	298.15	NIST Webbook
dvisc	0.0004273	Pa×s	331.14	Joback Method
dvisc	0.0003106	Pa×s	366.57	Joback Method
dvisc	0.0050451	Pa×s	189.43	Joback Method
dvisc	0.0002389	Pa×s	402.00	Joback Method
dvisc	0.0010493	Pa×s	260.29	Joback Method
dvisc	0.0006345	Pa×s	295.72	Joback Method
dvisc	0.0020331	Pa×s	224.86	Joback Method
hfust	19.97	kJ/mol	191.60	NIST Webbook
hfust	19.97	kJ/mol	191.60	NIST Webbook
hvapt	42.00	kJ/mol	381.00	NIST Webbook
hvapt	36.32	kJ/mol	420.00	KDB
rfi	1.41333		298.15	KDB
rhol	745.00	kg/m3	273.00	KDB
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44429e+01
Coeff. B	-3.57259e+03
Coeff. C	-5.53600e+01
Temperature range (K), min.	307.75
Temperature range (K), max.	446.60

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.06010e+02
Coeff. B	-9.03620e+03
Coeff. C	-1.34814e+01
Coeff. D	8.71053e-06
Temperature range (K), min.	191.78
Temperature range (K), max.	593.25

Sources

Separation of (water/butan-1-ol) binary systems based on activity coefficients at infinite dilution with phosphonium ionic liquid.	https://www.doi.org/10.1016/j.jct.2019.05.011
Screening of environmental friendly ionic liquid as a solvent for the separation of azeotropic problem: Insight from activity coefficients at infinite dilution.	https://www.doi.org/10.1016/j.jct.2015.08.017
Measurement of activity coefficients at infinite dilution of organic solutes in 1-hexadecyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ionic liquid using gas-liquid chromatography.	https://www.doi.org/10.1016/j.jct.2013.10.017
Activity coefficients at infinite dilution measurement using GLC.	https://www.doi.org/10.1016/j.jct.2009.08.012
Activity coefficients at infinite dilution for solutes chromatographed on the ionic liquid 1-hexadecyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide using gas-liquid chromatography at T = (313.15, 328.15, 343.15, 358.15, 373.15) K.	https://www.doi.org/10.1016/j.jct.2009.12.004
Activity coefficients at infinite dilution measurements using GLC method at T = (323.15 and 353.15) K.	https://www.doi.org/10.1016/j.fluid.2019.03.023
Activity coefficients at infinite dilution for solutes chromatographed on the ionic liquid 1-hexadecyl-3-methylimidazolium hexafluorophosphate using gas-liquid chromatography at T = (313.15, 328.15, 343.15, 358.15, 373.15) K.	https://www.doi.org/10.1016/j.jct.2010.12.019
Activity coefficients at infinite dilution measurements using GLC method.	http://link.springer.com/article/10.1007/BF02311772
Activity coefficients at infinite dilution for solutes chromatographed on the ionic liquid 1-hexadecyl-3-methylimidazolium hexafluoroantimonate using gas-liquid chromatography at T = (313.15, 323.15, and 333.15) K:	https://www.cheric.org/files/research/kdb/mol/mol341.mol
Activity coefficients at infinite dilution of hydrocarbons in glycols: Experimental data and thermodynamic modeling with the GCA-EOS.	https://www.doi.org/10.1016/j.jct.2016.10.013
Activity coefficients at infinite dilution of organic solutes in the ionic liquid tri-n-hexyl(tetradecyl)phosphonium tetrafluoroborate using gas-liquid chromatography at T = (313.15, 333.15, 353.15, and 373.15) K:	https://www.doi.org/10.1016/j.jct.2010.12.005
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C124118&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Infinite dilution activity coefficients, specific retention volumes and solvation thermodynamics of hydrocarbons in C78H158 branched alkane solvent.	https://www.doi.org/10.1016/j.fluid.2006.07.015
Cripps Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Assessment of Pyrrolidinium-Based Ionic Liquid for the Separation of Binary Mixtures Based on Activity Coefficients at Infinite Dilution of Hydrocarbons, Alcohols, Esters, and Aldehydes in Infinite Dilution of Hydrocarbons, Alcohols, Esters, and Aldehydes in	https://www.doi.org/10.1021/acs.jced.9b00341
Thermodynamic Properties of Mixtures Containing Ionic Liquids. 9. Activity Coefficients at Infinite Dilution of Hydrocarbons, Alcohols, Esters, and Aldehydes in	https://www.doi.org/10.1021/je050440b
Thermodynamic Properties of Mixtures Containing Ionic Liquids. 6. Activity Coefficients at Infinite Dilution of Hydrocarbons, Alcohols, Esters, and Aldehydes in	https://www.doi.org/10.1021/je050134y
Measurements of infinite dilution thermodynamic properties of systems containing ionic liquids and hydrocarbons	https://www.doi.org/10.1016/j.fluid.2010.02.010
Activity coefficients at infinite dilution measurements on 1-hexadecyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ionic liquid using gas-liquid chromatography and correlation with the GCA-EOS.	https://www.doi.org/10.1016/j.jct.2009.07.010
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Activity coefficients at infinite dilution for solutes in the ionic liquid 1-hexadecyl-3-methylimidazolium trifluoromethanesulfonate using gas-liquid chromatography at T = (313.15, 328.15, 343.15, 358.15, and 373.15) K.	https://www.doi.org/10.1021/je050125p
Thermodynamic Properties of Mixtures Containing Ionic Liquids. 5. Activity Coefficients at Infinite Dilution of Hydrocarbons, Alcohols, Esters, and Aldehydes in	https://www.doi.org/10.1021/je0503554
Joback Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=341
Activity coefficients at infinite dilution measurements on 1-hexadecyl-3-methyl-sulfonyl) imide.	https://www.doi.org/10.1016/j.jct.2012.01.004
Solubility Parameter Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Bis(trifluoromethylsulfonyl) imide hexafluorophosphate using gas-liquid chromatography at T = (313.15, 333.15, 353.15, and 363.15) K:	

Legend

af:	Acentric Factor
ap:	Aniline Point
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hcg:	Heat of Combustion, Gross form
hcn:	Heat of Combustion, Net Form
hf:	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
nfpaf:	NFPA Fire Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter