1-NONENE

Other names:	1-C9H18
	NSC 73961
	Non-1-ene
	Nonene-(1)
	Nonylene
	n-Non-1-ene
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	0.4055		Cheméo Relay (1.0)
gf	112.74	kJ/mol	Joback Method
hf	-107.74	kJ/mol	Cheméo Relay (1.0)
hfus	17.79	kJ/mol	Joback Method
hvap	45.50	kJ/mol	NIST Webbook
hvap	44.70 ± 0.20	kJ/mol	NIST Webbook
ie	9.42 ± 0.01	eV	NIST Webbook
log10ws	-5.05		Aqueous Solubility Prediction Method
log10ws	-5.05		Estimated Solubility Method
logp	3.533		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
rhoc	239.85	kg/m3	NIST Webbook
rinpol	889.50		NIST Webbook
rinpol	891.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	888.92		NIST Webbook
rinpol	889.50		NIST Webbook
rinpol	890.20		NIST Webbook
rinpol	883.00		NIST Webbook

rinpol	892.00	NIST Webbook
rinpol	888.80	NIST Webbook
rinpol	891.00	NIST Webbook
rinpol	895.00	NIST Webbook
rinpol	894.00	NIST Webbook
rinpol	890.00	NIST Webbook
rinpol	889.00	NIST Webbook
rinpol	884.00	NIST Webbook
rinpol	889.00	NIST Webbook
rinpol	896.00	NIST Webbook
rinpol	887.00	NIST Webbook
rinpol	879.00	NIST Webbook
rinpol	889.00	NIST Webbook
rinpol	888.00	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	891.00	NIST Webbook
rinpol	882.00	NIST Webbook
rinpol	889.00	NIST Webbook
rinpol	880.00	NIST Webbook
rinpol	889.00	NIST Webbook
rinpol	887.00	NIST Webbook
rinpol	888.00	NIST Webbook
rinpol	892.00	NIST Webbook
rinpol	899.00	NIST Webbook
rinpol	884.00	NIST Webbook
rinpol	890.00	NIST Webbook
rinpol	886.00	NIST Webbook
rinpol	888.80	NIST Webbook
rinpol	886.00	NIST Webbook
rinpol	886.00	NIST Webbook
rinpol	888.00	NIST Webbook
rinpol	886.00	NIST Webbook
rinpol	891.00	NIST Webbook
rinpol	886.00	NIST Webbook
rinpol	880.00	NIST Webbook
rinpol	892.00	NIST Webbook
rinpol	895.00	NIST Webbook
rinpol	893.00	NIST Webbook
rinpol	892.00	NIST Webbook
rinpol	892.00	NIST Webbook
rinpol	885.00	NIST Webbook
rinpol	882.00	NIST Webbook
rinpol	889.00	NIST Webbook
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rinpol	881.00	NIST Webbook
rinpol	885.20	NIST Webbook
rinpol	882.00	NIST Webbook
rinpol	886.00	NIST Webbook
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rinpol	889.00	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
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rinpol	883.40	NIST Webbook
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rinpol	881.00	NIST Webbook
rinpol	882.00	NIST Webbook
rinpol	883.00	NIST Webbook
rinpol	882.00	NIST Webbook
rinpol	889.00	NIST Webbook
rinpol	890.30	NIST Webbook
rinpol	882.70	NIST Webbook
rinpol	883.00	NIST Webbook
rinpol	882.80	NIST Webbook
rinpol	896.00	NIST Webbook
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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	882.20		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
ripol	949.70		NIST Webbook
ripol	950.50		NIST Webbook
ripol	923.00		NIST Webbook
ripol	929.00		NIST Webbook
ripol	930.00		NIST Webbook
ripol	930.00		NIST Webbook
ripol	949.80		NIST Webbook
ripol	931.00		NIST Webbook
ripol	947.70		NIST Webbook
ripol	952.00		NIST Webbook
ripol	960.00		NIST Webbook
ripol	950.00		NIST Webbook
ripol	929.00		NIST Webbook
ripol	953.00		NIST Webbook
ripol	950.50		NIST Webbook
ripol	949.80		NIST Webbook
ripol	950.00		NIST Webbook
ripol	946.00		NIST Webbook
sl	392.54	J/mol×K	NIST Webbook
tb	422.15 ± 1.00	K	NIST Webbook
tb	417.90 ± 0.30	K	NIST Webbook
tb	413.00 ± 5.00	K	NIST Webbook
tb	418.50 ± 1.50	K	NIST Webbook
tb	419.99 ± 0.20	K	NIST Webbook
tb	418.80 ± 0.80	K	NIST Webbook
tb	420.40 ± 1.50	K	NIST Webbook

tb	420.00 ± 4.00	K	NIST Webbook
tb	419.10 ± 2.50	K	NIST Webbook
tb	418.00 ± 3.00	K	NIST Webbook
tb	418.00 ± 20.00	K	NIST Webbook
tb	420.00 ± 1.50	K	NIST Webbook
tb	419.51 ± 0.40	K	NIST Webbook
tb	420.10	K	NIST Webbook
tc	594.00 ± 1.00	K	NIST Webbook
tf	192.06 ± 0.15	K	NIST Webbook
tf	191.40 ± 1.00	K	NIST Webbook
tf	191.33	K	Aqueous Solubility Prediction Method
tf	191.74 ± 0.06	K	NIST Webbook
tf	191.78 ± 0.03	K	NIST Webbook
tf	189.60 ± 2.00	K	NIST Webbook
tf	185.00 ± 1.50	K	NIST Webbook
tf	185.00 ± 5.00	K	NIST Webbook
tt	191.91 ± 0.00	K	NIST Webbook
tt	191.60 ± 0.00	K	NIST Webbook
tt	191.91 ± 0.00	K	NIST Webbook
tt	191.60 ± 0.00	K	NIST Webbook
vc	0.526	m3/kmol	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.25	J/mol×K	540.58	Joback Method
cpg	308.66	J/mol×K	512.86	Joback Method
cpg	296.58	J/mol×K	485.15	Joback Method
cpg	331.38	J/mol×K	568.30	Joback Method
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
cpl	270.36	J/mol×K	298.15	NIST Webbook
dvisc	0.0020331	Pa×s	224.86	Joback Method
dvisc	0.0050451	Pa×s	189.43	Joback Method
dvisc	0.0010493	Pa×s	260.29	Joback Method
dvisc	0.0006345	Pa×s	295.72	Joback Method
dvisc	0.0004273	Pa×s	331.14	Joback Method
dvisc	0.0003106	Pa×s	366.57	Joback Method
dvisc	0.0002389	Pa×s	402.00	Joback Method

hfust	19.97	kJ/mol	191.60	NIST Webbook
hfust	19.97	kJ/mol	191.60	NIST Webbook
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

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

Screening of environmental friendly ionic liquid as a solvent for the	https://www.doi.org/10.1016/j.jct.2015.08.017
Activity coefficients at infinite dilution of organic solutes in the ionic liquid	https://www.doi.org/10.1016/j.jct.2012.01.004
Thermodynamic Properties of Mixtures	https://www.doi.org/10.1021/je050125p
Containing Ionic Liquids. 6. Activity	https://www.doi.org/10.1016/j.jct.2009.08.012
Thermodynamic Properties of Mixtures	https://www.doi.org/10.1021/je050440b
Containing Ionic Liquids. 9. Activity	https://www.doi.org/10.1021/je0503554
Activity coefficients at infinite dilution of organic solutes in the ionic liquid	https://www.doi.org/10.1016/j.jct.2009.07.010

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C124118&Units=SI
Measurement of activity coefficients at infinite dilution of organic solutes in the ionic liquid	https://www.doi.org/10.1016/j.jct.2013.10.017
Application of	https://www.doi.org/10.1016/j.fluid.2019.03.023
1-ethyl-3-methylimidazolium	https://www.doi.org/10.1016/j.jct.2010.12.019
Activity coefficients at infinite dilution	https://www.doi.org/10.1021/je050368h
Determination of	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Activity coefficients at infinite dilution of organic solutes in the ionic liquid	https://www.doi.org/10.1016/j.jct.2009.12.004
Activity coefficients at infinite dilution	https://www.doi.org/10.1016/j.jct.2010.12.005
Thermodynamic Properties of Mixtures	https://www.doi.org/10.1021/je050134y
KDB/Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=341
Infinite dilution activity coefficients,	https://www.doi.org/10.1016/j.fluid.2006.07.015
2-Methyl-3-octyl-imidazolium	https://www.doi.org/10.1016/j.jct.2019.05.011
Joback Method	https://en.wikipedia.org/wiki/Joback_method
Assessment of Pyrrolidinium-Based Ionic Liquid for the Separation of	https://www.doi.org/10.1021/acs.jced.9b00341
Gripper Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/files/research/kdb/mol/mol341.mol
Activity coefficients at infinite dilution of hydrocarbons in glycols:	https://www.doi.org/10.1016/j.jct.2016.10.013
Experimental data and thermodynamic	https://www.doi.org/10.1016/j.fluid.2010.02.010
McGowan Method GCA EOS:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
UNIFAC (Dortmund):	
Cheméo Relay (1.0):	

Legend

af:	Acentric Factor
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
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
pc:	Critical Pressure
pvap:	Vapor pressure

rhoc:	Critical density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume