1-Octene

Other names:	1-C8H16
	1-n-Octene
	CAPRYLENE
	N-1-OCTENE
	NSC 8457
	Neodene 8
	Oct-1-ene
	Octene-1
	Octylene
	SHOP C8
	«alpha»-Octene
	«alpha»-Octylene
	Â«alphaÂ»-Octene
	Â«alphaÂ»-Octylene
Inchi:	InChI=1S/C8H16/c1-3-5-7-8-6-4-2/h3H,1,4-8H2,2H3
InchiKey:	KWKAKUADMBZCLK-UHFFFAOYSA-N
Formula:	C8H16
SMILES:	C=CCCCCCC
Mol. weight [g/mol]:	112.21
CAS:	111-66-0

Physical Properties

Property code	Value	Unit	Source
af	0.3860		KDB
aigt	529.26	K	KDB
ap	305.650	K	KDB
chl	-5312.90 ± 1.10	kJ/mol	NIST Webbook
dm	0.30	debye	KDB
fll	0.90	% in Air	KDB
fpc	294.26	K	KDB
gf	104.30	kJ/mol	KDB
hcg	5312.93	kJ/mol	KDB
hcn	4960.844	kJ/mol	KDB
hf	-82.93	kJ/mol	NIST Webbook
hf	-82.93	kJ/mol	NIST Webbook
hf	-82.98	kJ/mol	KDB
hfl	-121.80 ± 1.20	kJ/mol	NIST Webbook

hfus	15.20	kJ/mol	Joback Method
hvap	38.00	kJ/mol	NIST Webbook
hvap	40.60	kJ/mol	NIST Webbook
hvap	40.44	kJ/mol	NIST Webbook
hvap	40.30 ± 0.20	kJ/mol	NIST Webbook
hvap	40.27 ± 0.20	kJ/mol	NIST Webbook
ie	9.43 ± 0.01	eV	NIST Webbook
ie	9.43 ± 0.01	eV	NIST Webbook
ie	9.43 ± 0.01	eV	NIST Webbook
ie	9.60 ± 0.01	eV	NIST Webbook
log10ws	-4.44		Aqueous Solubility Prediction Method
log10ws	-4.44		Estimated Solubility Method
logp	3.143		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=1)		KDB
pc	2680.00 ± 80.00	kPa	NIST Webbook
pc	2680.00	kPa	KDB
rhoc	235.65 ± 8.98	kg/m3	NIST Webbook
rinpol	792.60		NIST Webbook
rinpol	786.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	786.00		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	790.00		NIST Webbook
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rinpol	789.00		NIST Webbook
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rinpol	789.00		NIST Webbook
rinpol	789.00		NIST Webbook
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rinpol	789.00	NIST Webbook
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rinpol	781.80	NIST Webbook
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rinpol	788.99	NIST Webbook
rinpol	789.05	NIST Webbook
rinpol	791.72	NIST Webbook
rinpol	791.76	NIST Webbook
rinpol	791.77	NIST Webbook
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ripol	830.00	NIST Webbook
ripol	830.00	NIST Webbook
ripol	822.00	NIST Webbook
ripol	850.00	NIST Webbook
ripol	892.00	NIST Webbook
ripol	837.00	NIST Webbook
ripol	836.00	NIST Webbook
ripol	833.00	NIST Webbook

ripol	837.00		NIST Webbook
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ripol	847.40		NIST Webbook
ripol	848.50		NIST Webbook
ripol	847.20		NIST Webbook
ripol	849.90		NIST Webbook
ripol	852.00		NIST Webbook
ripol	847.40		NIST Webbook
ripol	848.50		NIST Webbook
ripol	850.00		NIST Webbook
ripol	847.00		NIST Webbook
ripol	851.00		NIST Webbook
ripol	847.20		NIST Webbook
ripol	836.00		NIST Webbook
sl	360.45	J/mol×K	NIST Webbook
tb	394.44	K	KDB
tc	567.00 ± 0.80	K	NIST Webbook
tc	567.00	K	KDB
tc	566.55 ± 0.05	K	NIST Webbook
tc	566.60	K	NIST Webbook
tf	171.09 ± 0.10	K	NIST Webbook
tf	171.05 ± 0.40	K	NIST Webbook
tf	167.15 ± 1.50	K	NIST Webbook
tf	171.20 ± 1.00	K	NIST Webbook
tf	171.44 ± 0.03	K	NIST Webbook
tf	171.43 ± 0.05	K	NIST Webbook
tf	171.31 ± 0.20	K	NIST Webbook
tf	171.25	K	Aqueous Solubility Prediction Method
tf	171.40	K	KDB
tf	171.04 ± 0.30	K	NIST Webbook
tf	171.44 ± 0.03	K	NIST Webbook
tf	171.40 ± 0.06	K	NIST Webbook
tt	171.46 ± 0.05	K	NIST Webbook
vc	0.468	m3/kmol	KDB
vc	0.468	m3/kmol	NIST Webbook
zc	0.2660490		KDB
zra	0.26		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.22	J/mol×K	406.91	Joback Method
cpg	285.74	J/mol×K	545.88	Joback Method
cpg	275.52	J/mol×K	518.08	Joback Method
cpg	264.86	J/mol×K	490.29	Joback Method
cpg	253.77	J/mol×K	462.50	Joback Method
cpg	242.23	J/mol×K	434.71	Joback Method
cpg	217.72	J/mol×K	379.12	Joback Method
cpl	241.21	J/mol×K	298.15	NIST Webbook
dvisc	0.0003074	Pa×s	345.63	Joback Method
dvisc	0.0046461	Pa×s	178.16	Joback Method
dvisc	0.0019138	Pa×s	211.65	Joback Method
dvisc	0.0010045	Pa×s	245.15	Joback Method
dvisc	0.0006156	Pa×s	278.64	Joback Method
dvisc	0.0004191	Pa×s	312.13	Joback Method
dvisc	0.0002381	Pa×s	379.12	Joback Method
hfust	15.31	kJ/mol	171.46	NIST Webbook
hfust	15.31	kJ/mol	171.50	NIST Webbook
hfust	15.31	kJ/mol	171.50	NIST Webbook
hvapt	40.20	kJ/mol	277.00	NIST Webbook
hvapt	34.07	kJ/mol	394.40	NIST Webbook
hvapt	38.80	kJ/mol	356.00	NIST Webbook
hvapt	39.50 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	38.60 ± 0.10	kJ/mol	328.00	NIST Webbook
hvapt	37.60 ± 0.10	kJ/mol	343.00	NIST Webbook
hvapt	41.20	kJ/mol	275.50	NIST Webbook
hvapt	36.60 ± 0.10	kJ/mol	358.00	NIST Webbook
hvapt	33.77	kJ/mol	395.20	KDB
hvapt	35.80 ± 0.10	kJ/mol	368.00	NIST Webbook
pvap	10.12	kPa	328.15	Vapor Liquid Equilibrium and Excess Enthalpy Data for Systems Containing N,N-Dimethylacetamide
pvap	39.20	kPa	363.15	Vapor Liquid Equilibrium and Excess Enthalpy Data for Systems Containing N,N-Dimethylacetamide

pvap	53.82	kPa	373.10	Phase Equilibria on Four Binary Systems: 1,2-Dichloroethane + trans-1,2-Dichloroethylene, 1-Octene + 2-Methyl Thiophene, 2-Ethyl Thiophene + 2,2,4-Trimethylpentane, and Cyclopropanecarbonitrile + Water
pvap	165.90	kPa	413.15	Phase Equilibria on Four Binary Systems: 1,2-Dichloroethane + trans-1,2-Dichloroethylene, 1-Octene + 2-Methyl Thiophene, 2-Ethyl Thiophene + 2,2,4-Trimethylpentane, and Cyclopropanecarbonitrile + Water
pvap	8.30	kPa	323.15	Isothermal Phase Equilibria and Excess Molar Enthalpies for Binary Systems with Dimethyl Ether at 323.15 K
pvap	38.51	kPa	363.15	Measurement of vapor.liquid equilibria (VLE) and excess enthalpies (HE) of binary systems with 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide and prediction of these properties and A using modified UNIFAC (Dortmund)
rfi	1.40620		298.15	KDB

rhol	710.88	kg/m3	298.15	Excess molar enthalpy of 1-alkanol + 1-octene mixtures at 298.15K Experimental results and theoretical description by means of the ERAS and TB models
rhol	715.00	kg/m3	293.00	KDB
sdco	2.28e-07	m2/s	298.15	Viscosity and Diffusivity for the Ionic Liquid 1-Hexyl-3-methyl-imidazolium Bis(trifluoromethylsulfonyl)amide with 1-Octene
sdco	3.44e-07	m2/s	323.15	Viscosity and Diffusivity for the Ionic Liquid 1-Hexyl-3-methyl-imidazolium Bis(trifluoromethylsulfonyl)amide with 1-Octene
sfust	89.31	J/mol×K	171.46	NIST Webbook
srf	0.02	N/m	323.15	Phase Equilibrium, Volumetric, and Interfacial Properties of the Ionic Liquid, 1-Hexyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)amide and 1-Octene
srf	0.02	N/m	283.10	Phase Equilibrium, Volumetric, and Interfacial Properties of the Ionic Liquid, 1-Hexyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)amide and 1-Octene
srf	0.02	N/m	298.20	KDB
srf	0.02	N/m	348.15	Phase Equilibrium, Volumetric, and Interfacial Properties of the Ionic Liquid, 1-Hexyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)amide and 1-Octene

srf	0.02	N/m	298.15	Phase Equilibrium, Volumetric, and Interfacial Properties of the Ionic Liquid, 1-Hexyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)amide and 1-Octene
tcondl	0.12	W/m×K	326.44	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	326.70	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	326.87	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	316.24	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.12	W/m×K	316.07	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.12	W/m×K	315.82	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.12	W/m×K	297.28	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.12	W/m×K	297.14	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.12	W/m×K	296.88	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	

tcondl	0.13	W/m×K	279.72	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.13	W/m×K	279.57	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.13	W/m×K	279.34	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.14	W/m×K	260.06	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.14	W/m×K	259.90	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	

tcondl	0.14	W/m×K	259.69	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42819e+01
Coeff. B	-3.35220e+03
Coeff. C	-4.81090e+01
Temperature range (K), min.	287.65
Temperature range (K), max.	421.80

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.67823e+01
Coeff. B	-8.07486e+03
Coeff. C	-1.22214e+01
Coeff. D	8.73474e-06
Temperature range (K), min.	171.45
Temperature range (K), max.	566.60

Datasets

Thermal conductivity, W/m/K

Temperature, K - Liquid	Pressure, kPa - Liquid	Thermal conductivity, W/m/K - Liquid
254.47	100.00	0.1381
254.41	5000.00	0.1402
254.47	10000.00	0.1426
254.35	20000.00	0.1464
254.35	30000.00	0.1500
274.46	100.00	0.1302
274.44	5000.00	0.1324
274.50	10000.00	0.1349
274.59	20000.00	0.1394
274.44	30000.00	0.1439
294.91	100.00	0.1254
294.90	5200.00	0.1277
294.85	10100.00	0.1300
294.79	20000.00	0.1341
294.76	30000.00	0.1379
314.65	100.00	0.1200
314.61	5000.00	0.1228
314.59	10000.00	0.1249
314.61	20000.00	0.1291
314.51	30000.00	0.1331
334.94	100.00	0.1140
334.82	5100.00	0.1167
334.82	10000.00	0.1191
334.69	20000.00	0.1238
334.71	30000.00	0.1282
355.05	100.00	0.1078
354.89	5100.00	0.1106
354.72	10000.00	0.1137
354.74	20000.00	0.1186
354.64	30000.00	0.1234
374.48	600.00	0.1023
375.03	5100.00	0.1047
374.83	10000.00	0.1077
374.86	20100.00	0.1135
374.80	30000.00	0.1179

Reference *https://www.doi.org/10.1021/acs.jced.9b00628*

Sources

Activity coefficients at infinite dilution and physicochemical properties for [illegible]	https://www.doi.org/10.1016/j.jct.2012.03.015
Determination of Activity Coefficients at Infinite Dilution of Solutes in [illegible]	https://www.doi.org/10.1021/acs.jced.8b00635
Activity coefficients at infinite dilution [illegible]	https://www.doi.org/10.1016/j.jct.2010.12.005
[illegible]	https://www.doi.org/10.1016/j.jct.2015.08.017
[illegible]	http://link.springer.com/article/10.1007/BF02311772
Activity coefficients at infinite dilution of organic solutes in the ionic liquid [illegible]	https://www.doi.org/10.1016/j.jct.2009.12.004
Measurements of activity coefficients at infinite dilution of aromatic and [illegible]	https://www.doi.org/10.1016/j.jct.2008.01.004
Activity coefficients at infinite dilution measurements for organic solutes in [illegible]	https://www.doi.org/10.1016/j.jct.2005.01.015
Activity Coefficients at Infinite Dilution of Organic Solutes in [illegible]	https://www.doi.org/10.1021/je0256481
Activity coefficients at infinite dilution for solutes in the [illegible]	https://www.doi.org/10.1016/j.jct.2009.08.012
Activity coefficients at infinite dilution, physicochemical and thermodynamic properties for organic solutes and water in the ionic liquid [illegible]	https://www.doi.org/10.1016/j.jct.2015.05.022
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=249
Interactions of Volatile Organic Compounds with the Ionic Liquid [illegible]	https://www.doi.org/10.1021/je200822w
KDB	https://www.cheric.org/files/research/kdb/mol/mol249.mol
Solubilities of the Gaseous and Liquid Solutes and Their Thermodynamics of Solubilization in the Novel Room-Temperature Ionic Liquids at Infinite Dilution by Gas Chromatography	https://www.doi.org/10.1021/je700297c
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Activity coefficients at infinite dilution of organic solutes in the ionic liquid [illegible]	https://www.doi.org/10.1016/j.jct.2012.01.004
Activity coefficients at infinite dilution and physicochemical properties for [illegible]	https://www.doi.org/10.1016/j.jct.2015.02.024
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[illegible]	https://www.doi.org/10.1016/j.fluid.2006.07.015
Measurement of activity coefficients at infinite dilution of organic solutes in [illegible]	https://www.doi.org/10.1016/j.jct.2013.10.017
[illegible] coefficients at infinite dilution [illegible]	https://www.doi.org/10.1016/j.fluid.2016.02.004
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[illegible]	https://www.doi.org/10.1016/j.jct.2018.07.024
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Legend

af:	Acentric Factor
aigt:	Autoignition Temperature
ap:	Aniline Point
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
fll:	Lower Flammability Limit
fpc:	Flash Point (Closed Cup Method)
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
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health 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
sdco:	Self diffusion coefficient
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions

srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter