1-Undecene

Other names:	N-1-UNDECENE
	Undec-1-ene
	Undecene-1
	«alpha»-Undecene
	Â«alphaÂ»-Undecene
Inchi:	InChI=1S/C11H22/c1-3-5-7-9-11-10-8-6-4-2/h3H,1,4-11H2,2H3
InchiKey:	DCTOHCCUXLBQMS-UHFFFAOYSA-N
Formula:	C11H22
SMILES:	C=CCCCCCCCCC
Mol. weight [g/mol]:	154.29
CAS:	821-95-4

Physical Properties

Property code	Value	Unit	Source
af	0.5180		KDB
gf	129.50	kJ/mol	KDB
hf	-144.90	kJ/mol	KDB
hfus	22.97	kJ/mol	Joback Method
hvap	55.40	kJ/mol	NIST Webbook
hvap	54.30 ± 0.30	kJ/mol	NIST Webbook
log10ws	-4.28		Crippen Method
logp	4.313		Crippen Method
mcvol	161.550	ml/mol	McGowan Method
pc	1990.00	kPa	KDB
rinpol	1090.00		NIST Webbook
rinpol	1089.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1089.90		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1088.00		NIST Webbook

rinpol	1090.00	NIST Webbook
rinpol	1090.50	NIST Webbook
rinpol	1093.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1088.00	NIST Webbook
rinpol	1088.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1087.00	NIST Webbook
rinpol	1090.90	NIST Webbook
rinpol	1091.40	NIST Webbook
rinpol	1091.40	NIST Webbook
rinpol	1086.00	NIST Webbook
rinpol	1090.90	NIST Webbook
rinpol	1091.40	NIST Webbook
rinpol	1091.40	NIST Webbook
rinpol	1089.00	NIST Webbook
rinpol	1088.00	NIST Webbook
rinpol	1088.79	NIST Webbook
rinpol	1088.78	NIST Webbook
rinpol	1088.91	NIST Webbook
rinpol	1091.72	NIST Webbook
rinpol	1091.85	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1088.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1093.00	NIST Webbook
rinpol	1093.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1089.00	NIST Webbook
rinpol	1089.00	NIST Webbook
rinpol	1091.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1091.00	NIST Webbook
rinpol	1089.00	NIST Webbook
rinpol	1095.00	NIST Webbook
rinpol	1088.60	NIST Webbook
rinpol	1089.00	NIST Webbook
rinpol	1088.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1088.00	NIST Webbook
rinpol	1097.00	NIST Webbook
rinpol	1100.00	NIST Webbook

rinpol	1086.00	NIST Webbook
rinpol	1090.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1090.00	NIST Webbook
rinpol	1082.00	NIST Webbook
rinpol	1087.00	NIST Webbook
rinpol	1089.00	NIST Webbook
rinpol	1088.00	NIST Webbook
rinpol	1082.00	NIST Webbook
rinpol	1083.00	NIST Webbook
rinpol	179.50	NIST Webbook
rinpol	1093.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1095.00	NIST Webbook
rinpol	1088.00	NIST Webbook
rinpol	179.50	NIST Webbook
rinpol	1090.90	NIST Webbook
rinpol	1088.79	NIST Webbook
rinpol	1084.00	NIST Webbook
rinpol	1093.00	NIST Webbook
ripol	1135.00	NIST Webbook
ripol	1154.00	NIST Webbook
ripol	1148.00	NIST Webbook
ripol	1146.00	NIST Webbook
ripol	1146.00	NIST Webbook
ripol	1146.00	NIST Webbook
ripol	1147.00	NIST Webbook
ripol	1145.00	NIST Webbook
ripol	1151.20	NIST Webbook
ripol	1153.60	NIST Webbook
ripol	1148.40	NIST Webbook
ripol	1151.20	NIST Webbook
ripol	1153.60	NIST Webbook
ripol	1148.40	NIST Webbook
ripol	1147.00	NIST Webbook
ripol	1135.00	NIST Webbook
ripol	1142.00	NIST Webbook
ripol	1141.00	NIST Webbook
ripol	1151.00	NIST Webbook
ripol	1136.00	NIST Webbook
ripol	1139.00	NIST Webbook
ripol	1139.00	NIST Webbook
ripol	1138.00	NIST Webbook
ripol	1136.00	NIST Webbook

ripol	1152.00		NIST Webbook
ripol	1160.00		NIST Webbook
sl	456.56	J/mol×K	NIST Webbook
tb	465.80	K	KDB
tc	637.00	K	KDB
tf	224.00	K	KDB
tt	223.99 ± 0.01	K	NIST Webbook
tt	223.98 ± 0.05	K	NIST Webbook
vc	0.632	m3/kmol	KDB
zc	0.2376500		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.43	J/mol×K	612.57	Joback Method
cpg	373.51	J/mol×K	502.70	Joback Method
cpg	387.83	J/mol×K	530.16	Joback Method
cpg	401.58	J/mol×K	557.63	Joback Method
cpg	414.77	J/mol×K	585.10	Joback Method
cpg	343.08	J/mol×K	447.76	Joback Method
cpg	358.60	J/mol×K	475.23	Joback Method
cpl	329.95	J/mol×K	298.15	NIST Webbook
dvisc	0.0004159	Pa×s	369.16	Joback Method
dvisc	0.0006289	Pa×s	329.87	Joback Method
dvisc	0.0010633	Pa×s	290.57	Joback Method
dvisc	0.0021190	Pa×s	251.27	Joback Method
dvisc	0.0002262	Pa×s	447.76	Joback Method
dvisc	0.0002979	Pa×s	408.46	Joback Method
dvisc	0.0054528	Pa×s	211.97	Joback Method
hfust	16.99	kJ/mol	224.00	NIST Webbook
hfust	9.20	kJ/mol	217.30	NIST Webbook
hfust	16.99	kJ/mol	224.00	NIST Webbook
hvapt	48.20	kJ/mol	425.50	NIST Webbook
hvapt	40.88	kJ/mol	465.80	KDB
rhol	751.00	kg/m3	293.00	KDB
sfust	75.84	J/mol×K	224.00	NIST Webbook
sfust	42.36	J/mol×K	217.30	NIST Webbook
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44919e+01
Coeff. B	-3.90995e+03
Coeff. C	-6.99970e+01
Temperature range (K), min.	345.26
Temperature range (K), max.	495.90

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.36979e+02
Coeff. B	-1.16219e+04
Coeff. C	-1.78317e+01
Coeff. D	9.87600e-06
Temperature range (K), min.	223.99
Temperature range (K), max.	638.00

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol346.mol
Activity coefficients at infinite dilution of organic solutes in the ionic liquid 1-ethyl-3-methylimidazolium trifluoromethanesulfonate using gas liquid chromatography at T = (313.15, 323.15, and 333.15) K:	https://www.doi.org/10.1016/j.jct.2009.07.010
Thermodynamic Properties of Mixtures Containing Ionic Liquids. 8. Activity Coefficients at Infinite Dilution of Hydrocarbons, Alcohols, Esters, and Aldehydes in 1-Hexyl-3-methylimidazolium Bis(trifluoromethylsulfonyl) Imide Using Gas Liquid Chromatography:	https://www.doi.org/10.1021/je0503554
Crippen Method - Free Energy of Solvation:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C821954&Units=SI
Infinite dilution activity coefficients, specific retention volumes and solvation thermodynamics of hydrocarbons in C7H13O2 branched alkane solvent:	https://www.doi.org/10.1016/j.fluid.2006.07.015
Thermodynamic Properties of Mixtures Containing Ionic Liquids. 6. Activity Coefficients at Infinite Dilution of Hydrocarbons, Alcohols, Esters, and Aldehydes in 1-Hexyl-3-methylimidazolium Bis(trifluoromethylsulfonyl) Imide Using Gas-Liquid Chromatography:	https://www.doi.org/10.1021/je050134y
Thermodynamic Properties of Mixtures Containing Ionic Liquids. 9. Activity Coefficients at Infinite Dilution of Hydrocarbons, Alcohols, Esters, and Aldehydes in 1-Hexadecyl-3-methylimidazolium Tetrafluoroborate Using Gas-Liquid Chromatography:	https://www.doi.org/10.1021/je050440b
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
Thermodynamic Properties of Mixtures Containing Ionic Liquids. 5. Activity Coefficients at Infinite Dilution of Hydrocarbons, Alcohols, Esters, and Aldehydes in 1-Methyl-3-butyl-imidazolium Bis(trifluoromethyl-sulfonyl) Imide Using Gas-Liquid Chromatography and Static Method:	https://www.doi.org/10.1021/je050125p
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=346

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
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
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
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility