1-Dodecene

Other names:	Adacene 12
	Dodec-1-ene
	Dodecene-1
	Dodecylene «alpha»-
	Dodecylene Â«alphaÂ»-
	N-DODEC-1-ENE
	NSC 12016
	Neodene 12
	«alpha»-Dodecene
	«alpha»-Dodecylene
	Â«alphaÂ»-Dodecene
	Â«alphaÂ»-Dodecylene
Inchi:	InChI=1S/C12H24/c1-3-5-7-9-11-12-10-8-6-4-2/h3H,1,4-12H2,2H3
InchiKey:	CRSBERNSMYQZNG-UHFFFAOYSA-N
Formula:	C12H24
SMILES:	C=CCCCCCCCCC
Mol. weight [g/mol]:	168.32
CAS:	112-41-4

Physical Properties

Property code	Value	Unit	Source
af	0.5580		KDB
chl	-7925.90 ± 1.30	kJ/mol	NIST Webbook
gf	138.00	kJ/mol	KDB
hf	-165.50	kJ/mol	KDB
hf	-165.40 ± 2.10	kJ/mol	NIST Webbook
hf	-165.20	kJ/mol	NIST Webbook
hfl	-226.20 ± 2.10	kJ/mol	NIST Webbook
hfus	25.56	kJ/mol	Joback Method
hvap	60.78 ± 0.29	kJ/mol	NIST Webbook
hvap	60.30	kJ/mol	NIST Webbook
hvap	60.80 ± 0.30	kJ/mol	NIST Webbook
hvap	60.78 ± 0.20	kJ/mol	NIST Webbook
hvap	60.78	kJ/mol	NIST Webbook
log10ws	-4.70		Crippen Method
logp	4.703		Crippen Method
mcvol	175.640	ml/mol	McGowan Method

nfpaf	%!d(float64=1)		KDB
pc	1930.00 ± 200.00	kPa	NIST Webbook
pc	1930.00	kPa	KDB
rinpol	1188.00		NIST Webbook
rinpol	1187.90		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1183.00		NIST Webbook
rinpol	1183.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1190.10		NIST Webbook
rinpol	1183.00		NIST Webbook
rinpol	1183.40		NIST Webbook
rinpol	1183.80		NIST Webbook
rinpol	1182.50		NIST Webbook
rinpol	1189.00		NIST Webbook
rinpol	1192.20		NIST Webbook
rinpol	1193.00		NIST Webbook
rinpol	1192.00		NIST Webbook
rinpol	1189.00		NIST Webbook
rinpol	1187.00		NIST Webbook
rinpol	1191.30		NIST Webbook
rinpol	1191.30		NIST Webbook
rinpol	1191.30		NIST Webbook
rinpol	1186.00		NIST Webbook
rinpol	1195.00		NIST Webbook
rinpol	1187.00		NIST Webbook
rinpol	1191.30		NIST Webbook
rinpol	1191.30		NIST Webbook
rinpol	1191.30		NIST Webbook
rinpol	1193.00		NIST Webbook
rinpol	1188.76		NIST Webbook
rinpol	1188.93		NIST Webbook
rinpol	1189.04		NIST Webbook
rinpol	1191.75		NIST Webbook
rinpol	1191.82		NIST Webbook
rinpol	1192.15		NIST Webbook
rinpol	1189.00		NIST Webbook
rinpol	1190.00		NIST Webbook
rinpol	1192.00		NIST Webbook
rinpol	1193.00		NIST Webbook
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rinpol	1200.00	NIST Webbook
rinpol	1188.00	NIST Webbook
rinpol	1188.00	NIST Webbook
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rinpol	1199.00	NIST Webbook
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ripol	1249.00	NIST Webbook
ripol	1245.00	NIST Webbook
ripol	1235.10	NIST Webbook
ripol	1242.90	NIST Webbook
ripol	1236.30	NIST Webbook
ripol	1243.60	NIST Webbook
ripol	1231.60	NIST Webbook
ripol	1235.70	NIST Webbook
ripol	1241.90	NIST Webbook
ripol	1242.10	NIST Webbook
ripol	1232.20	NIST Webbook
ripol	1236.30	NIST Webbook
ripol	1242.50	NIST Webbook
ripol	1242.60	NIST Webbook
ripol	1251.00	NIST Webbook
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ripol	1252.80	NIST Webbook
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ripol	1246.00	NIST Webbook
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ripol	1255.00		NIST Webbook
ripol	1246.00		NIST Webbook
ripol	1240.60		NIST Webbook
ripol	1238.40		NIST Webbook
ripol	1236.00		NIST Webbook
ripol	1242.00		NIST Webbook
ripol	1244.20		NIST Webbook
sl	484.80	J/mol×K	NIST Webbook
tb	486.90	K	KDB
tc	658.00 ± 2.00	K	NIST Webbook
tc	658.00	K	KDB
tf	239.60 ± 0.50	K	NIST Webbook
tf	237.80 ± 0.20	K	NIST Webbook
tf	237.89 ± 0.05	K	NIST Webbook
tf	239.60 ± 2.00	K	NIST Webbook
tf	237.90	K	KDB
tf	237.75 ± 0.50	K	NIST Webbook
tf	237.88 ± 0.06	K	NIST Webbook
tf	237.89 ± 0.04	K	NIST Webbook
tf	237.92 ± 0.03	K	NIST Webbook
tf	237.92 ± 0.04	K	NIST Webbook
tf	237.92 ± 0.03	K	NIST Webbook
tt	237.93	K	KDB
tt	237.93 ± 0.05	K	NIST Webbook
vc	0.689	m3/kmol	KDB
zc	0.2428840		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.40	J/mol×K	607.24	Joback Method

cpg	477.70	J/mol×K	634.56	Joback Method
cpg	389.04	J/mol×K	470.64	Joback Method
cpg	405.36	J/mol×K	497.96	Joback Method
cpg	421.03	J/mol×K	525.28	Joback Method
cpg	436.09	J/mol×K	552.60	Joback Method
cpg	450.54	J/mol×K	579.92	Joback Method
cpl	360.66	J/mol×K	298.15	NIST Webbook
dvisc	0.0002149	Pa×s	470.64	Joback Method
dvisc	0.0054785	Pa×s	223.24	Joback Method
dvisc	0.0020968	Pa×s	264.47	Joback Method
dvisc	0.0010398	Pa×s	305.71	Joback Method
dvisc	0.0006092	Pa×s	346.94	Joback Method
dvisc	0.0003999	Pa×s	388.17	Joback Method
dvisc	0.0002846	Pa×s	429.41	Joback Method
hfust	19.87	kJ/mol	237.90	NIST Webbook
hfust	4.55	kJ/mol	212.90	NIST Webbook
hfust	19.87	kJ/mol	237.90	NIST Webbook
hvapt	51.10	kJ/mol	444.50	NIST Webbook
hvapt	42.97	kJ/mol	486.50	KDB
pvap	52.60	kPa	459.86	Isobaric vapor-liquid equilibrium for binary systems containing benzothiophene
pvap	61.60	kPa	464.81	Isobaric vapor-liquid equilibrium for binary systems containing benzothiophene
pvap	44.00	kPa	453.99	Isobaric vapor-liquid equilibrium for binary systems containing benzothiophene
pvap	80.80	kPa	476.45	Isobaric vapor-liquid equilibrium for binary systems containing benzothiophene
pvap	90.20	kPa	480.78	Isobaric vapor-liquid equilibrium for binary systems containing benzothiophene

pvap	100.70	kPa	484.11	Isobaric vapor-liquid equilibrium for binary systems containing benzothiophene
pvap	33.60	kPa	443.18	Isobaric vapor-liquid equilibrium for binary systems containing benzothiophene
pvap	21.70	kPa	430.38	Isobaric vapor-liquid equilibrium for binary systems containing benzothiophene
pvap	70.70	kPa	470.91	Isobaric vapor-liquid equilibrium for binary systems containing benzothiophene
rhol	758.00	kg/m3	293.00	KDB
sfust	83.54	J/mol×K	237.90	NIST Webbook
sfust	21.38	J/mol×K	212.90	NIST Webbook
srf	0.03	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47045e+01
Coeff. B	-4.19102e+03
Coeff. C	-7.06790e+01
Temperature range (K), min.	361.38
Temperature range (K), max.	516.86

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.28985e+02
Coeff. B	-1.18314e+04
Coeff. C	-1.64625e+01
Coeff. D	7.72637e-06

Temperature range (K), min.	237.93
Temperature range (K), max.	657.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112414&Units=SI
Isobaric vapor-liquid equilibrium for binary systems containing benzothiophene:	https://www.doi.org/10.1016/j.fluid.2011.04.024
Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=347
KDB:	https://www.cheric.org/files/research/kdb/mol/mol347.mol
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Modeling of Liquid Liquid Interfacial Properties of Binary and Ternary Mixtures:	https://www.doi.org/10.1021/je500113q
Thermodynamic Properties of Mixtures Containing Ionic Liquids. 6. Activity Coefficients at Infinite Dilution of Hydrocarbons, Alcohols, Esters, and Aldehydes in Tributyl-octylammonium Bis(trifluoromethylsulfonyl) Imide Using Gas-Liquid Chromatography:	https://www.doi.org/10.1021/je050134y
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermodynamic Properties of Mixtures Containing Ionic Liquids. 9. Activity Coefficients at Infinite Dilution of Hydrocarbons, Alcohols, Esters, and Aldehydes in Tributyl-octylammonium Bis(trifluoromethyl-sulfonyl) Imide Using Gas-Liquid Chromatography and Static Method:	https://www.doi.org/10.1021/je050440b
Thermodynamic Properties of Mixtures Containing Ionic Liquids. 1. Activity Coefficients at Infinite Dilution of Hydrocarbons, Alcohols, Esters, and Aldehydes in 1-Methyl-3-butyl-imidazolium Bis(trifluoromethylsulfonyl) Imide Using Gas-Liquid Chromatography:	https://www.doi.org/10.1021/je050125p

af:	Acentric Factor
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

nfpaf:	NFPA Fire Rating
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