Benzene, undecyl-

Other names:	1-PHENYLUNDECANE
	Phenylundecane
	UNDECANYLBENZENE
	Undecane, 1-phenyl-
	Undecylbenzene
	n-Undecylbenzene
Inchi:	InChI=1S/C17H28/c1-2-3-4-5-6-7-8-9-11-14-17-15-12-10-13-16-17/h10,12-13,15-16H,2-9
InchiKey:	XBEADGFTLHRJRB-UHFFFAOYSA-N
Formula:	C17H28
SMILES:	CCCCCCCCCCCc1ccccc1
Mol. weight [g/mol]:	232.40
CAS:	6742-54-7

Physical Properties

Property code	Value	Unit	Source
af	0.7220		KDB
gf	204.67	kJ/mol	Joback Method
hf	-157.68	kJ/mol	Joback Method
hfus	33.83	kJ/mol	Joback Method
hvap	84.70	kJ/mol	NIST Webbook
hvap	82.40 ± 0.40	kJ/mol	NIST Webbook
log10ws	-6.04		Crippen Method
logp	5.760		Crippen Method
mcvol	226.630	ml/mol	McGowan Method
pc	1670.00	kPa	KDB
rinpol	1760.12		NIST Webbook
rinpol	1765.33		NIST Webbook
rinpol	1779.75		NIST Webbook
rinpol	1785.43		NIST Webbook
rinpol	1789.05		NIST Webbook
rinpol	1769.12		NIST Webbook
tb	569.00 ± 4.00	K	NIST Webbook
tb	586.40	K	KDB
tc	764.00	K	KDB
tf	268.00	K	KDB
vc	0.910	m3/kmol	KDB
zc	0.2392370		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.41	J/mol×K	615.04	Joback Method
cpg	617.84	J/mol×K	646.25	Joback Method
cpg	636.28	J/mol×K	677.46	Joback Method
cpg	653.75	J/mol×K	708.68	Joback Method
cpg	670.31	J/mol×K	739.89	Joback Method
cpg	685.99	J/mol×K	771.10	Joback Method
cpg	700.83	J/mol×K	802.31	Joback Method
dvisc	0.0032077	Pa×s	307.77	Joback Method
dvisc	0.0013024	Pa×s	358.98	Joback Method
dvisc	0.0006623	Pa×s	410.19	Joback Method
dvisc	0.0003913	Pa×s	461.40	Joback Method
dvisc	0.0002568	Pa×s	512.62	Joback Method
dvisc	0.0001820	Pa×s	563.83	Joback Method
dvisc	0.0001366	Pa×s	615.04	Joback Method
hvapt	66.70	kJ/mol	536.00	NIST Webbook
hvapt	52.30	kJ/mol	586.40	KDB
pvap	2.70e-04	kPa	313.20	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	5.00e-04	kPa	319.30	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	7.20e-04	kPa	323.30	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	1.04e-03	kPa	327.30	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes

pvap	1.46e-03	kPa	331.30	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	1.76e-03	kPa	333.40	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	2.62e-03	kPa	338.40	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	4.13e-03	kPa	343.50	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	5.98e-03	kPa	348.70	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	9.06e-03	kPa	353.60	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	0.01	kPa	358.70	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	0.02	kPa	363.80	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tfp	256.90	K	100.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	261.40	K	20600.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	265.50	K	40400.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	269.70	K	60900.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	273.70	K	81000.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	277.10	K	99900.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54942e+01
Coeff. B	-5.32999e+03
Coeff. C	-9.26560e+01
Temperature range (K), min.	443.16
Temperature range (K), max.	616.09

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.00765e+02
Coeff. B	-1.82686e+04
Coeff. C	-2.64665e+01
Coeff. D	1.07638e-05
Temperature range (K), min.	268.00
Temperature range (K), max.	764.00

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
293.15	100.00	856.8
293.15	5000.00	859.6
293.15	10000.00	862.4
293.15	15000.00	865.1
293.15	20000.00	867.7
293.15	25000.00	870.3
293.15	30000.00	872.7
293.15	35000.00	875.2
293.15	40000.00	877.5
293.15	45000.00	879.8
293.15	50000.00	882.0
293.15	55000.00	884.2
293.15	60000.00	886.3
293.15	65000.00	888.2
303.15	100.00	849.5
303.15	5000.00	852.6
303.15	10000.00	855.4
303.15	15000.00	858.5
303.15	20000.00	861.1
303.15	25000.00	863.8
303.15	30000.00	866.3
303.15	35000.00	868.7
303.15	40000.00	871.2
303.15	45000.00	873.5

303.15	50000.00	875.8
303.15	55000.00	878.1
303.15	60000.00	880.3
303.15	65000.00	882.5
313.15	100.00	842.5
313.15	5000.00	845.7
313.15	10000.00	848.7
313.15	15000.00	851.6
313.15	20000.00	854.4
313.15	25000.00	857.2
313.15	30000.00	859.8
313.15	35000.00	862.4
313.15	40000.00	864.9
313.15	45000.00	867.5
313.15	50000.00	869.9
313.15	55000.00	872.3
313.15	60000.00	874.5
313.15	65000.00	876.8
323.15	100.00	835.5
323.15	5000.00	838.9
323.15	10000.00	842.1
323.15	15000.00	845.1
323.15	20000.00	848.1
323.15	25000.00	851.1
323.15	30000.00	853.9
323.15	35000.00	856.6
323.15	40000.00	859.2
323.15	45000.00	861.7
323.15	50000.00	864.2
323.15	55000.00	866.6
323.15	60000.00	869.0
323.15	65000.00	871.3
333.15	100.00	828.6
333.15	5000.00	831.9
333.15	10000.00	835.4
333.15	15000.00	838.6
333.15	20000.00	841.7
333.15	25000.00	844.6
333.15	30000.00	847.5
333.15	35000.00	850.3
333.15	40000.00	853.0
333.15	45000.00	855.7
333.15	50000.00	858.3
333.15	55000.00	860.9

333.15	60000.00	863.3
333.15	65000.00	865.6
343.15	100.00	821.7
343.15	5000.00	825.2
343.15	10000.00	828.7
343.15	15000.00	832.2
343.15	20000.00	835.4
343.15	25000.00	838.5
343.15	30000.00	841.4
343.15	35000.00	844.0
343.15	40000.00	846.8
343.15	45000.00	849.6
343.15	50000.00	852.3
343.15	55000.00	854.9
343.15	60000.00	857.4
343.15	65000.00	859.8
353.15	100.00	814.5
353.15	5000.00	818.5
353.15	10000.00	822.2
353.15	15000.00	825.9
353.15	20000.00	829.3
353.15	25000.00	832.5
353.15	30000.00	835.5
353.15	35000.00	838.4
353.15	40000.00	841.3
353.15	45000.00	844.1
353.15	50000.00	846.6
353.15	55000.00	849.4
353.15	60000.00	851.9
353.15	65000.00	854.6

Reference *https://www.doi.org/10.1021/je0500936*

Sources

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The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6742547&Units=SI
Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes:	https://www.doi.org/10.1021/je700529y
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas 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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tfp:	Melting point
vc:	Critical Volume
zc:	Critical Compressibility

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