Benzene, pentyl-

Other names:	1-PHENYLPENTANE
	1-Phenyl-n-pentane
	Amylbenzene
	Benzene, n-pentyl-
	N-AMYLBENZENE
	NSC 73982
	Pentane, 1-phenyl-
	Pentylbenzene
	Phenylpentane
	n-Pentylbenzene
Inchi:	InChI=1S/C11H16/c1-2-3-5-8-11-9-6-4-7-10-11/h4,6-7,9-10H,2-3,5,8H2,1H3
InchiKey:	PWATWSYOIIXYMA-UHFFFAOYSA-N
Formula:	C11H16
SMILES:	CCCCCc1ccccc1
Mol. weight [g/mol]:	148.24
CAS:	538-68-1

Physical Properties

Property code	Value	Unit	Source
af	0.4370		KDB
gf	154.15	kJ/mol	Joback Method
hf	-33.84	kJ/mol	Joback Method
hfus	18.29	kJ/mol	Joback Method
hvap	55.10 ± 0.40	kJ/mol	NIST Webbook
hvap	55.10	kJ/mol	NIST Webbook
hvap	55.30	kJ/mol	NIST Webbook
log10ws	-4.64		Aqueous Solubility Prediction Method
log10ws	-4.64		Estimated Solubility Method
logp	3.419		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2600.00	kPa	KDB
rinpol	1131.30		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1136.20		NIST Webbook

rinpol	1145.30	NIST Webbook
rinpol	1150.90	NIST Webbook
rinpol	1157.40	NIST Webbook
rinpol	1131.30	NIST Webbook
rinpol	1136.20	NIST Webbook
rinpol	1133.00	NIST Webbook
rinpol	1128.58	NIST Webbook
rinpol	1178.00	NIST Webbook
rinpol	1136.00	NIST Webbook
rinpol	1135.20	NIST Webbook
rinpol	1159.00	NIST Webbook
rinpol	1142.00	NIST Webbook
rinpol	1143.00	NIST Webbook
rinpol	1141.00	NIST Webbook
rinpol	1165.00	NIST Webbook
rinpol	1148.70	NIST Webbook
rinpol	1136.00	NIST Webbook
rinpol	1142.00	NIST Webbook
rinpol	1163.00	NIST Webbook
rinpol	1157.00	NIST Webbook
rinpol	1154.00	NIST Webbook
rinpol	1146.00	NIST Webbook
rinpol	1140.90	NIST Webbook
rinpol	1143.10	NIST Webbook
rinpol	1167.00	NIST Webbook
rinpol	1144.00	NIST Webbook
rinpol	1145.00	NIST Webbook
rinpol	1157.30	NIST Webbook
rinpol	1163.50	NIST Webbook
rinpol	1177.00	NIST Webbook
rinpol	1169.90	NIST Webbook
rinpol	1173.50	NIST Webbook
rinpol	1150.00	NIST Webbook
rinpol	1134.00	NIST Webbook
rinpol	1134.00	NIST Webbook
rinpol	1138.36	NIST Webbook
rinpol	1142.28	NIST Webbook
rinpol	1144.71	NIST Webbook
rinpol	1155.95	NIST Webbook
rinpol	1160.10	NIST Webbook
rinpol	1162.94	NIST Webbook
rinpol	1141.00	NIST Webbook
rinpol	1160.10	NIST Webbook
rinpol	1163.00	NIST Webbook

rinpol	1145.00	NIST Webbook
rinpol	1145.00	NIST Webbook
rinpol	1145.00	NIST Webbook
rinpol	1151.00	NIST Webbook
rinpol	1140.50	NIST Webbook
rinpol	1123.00	NIST Webbook
rinpol	1139.00	NIST Webbook
rinpol	1142.00	NIST Webbook
rinpol	1144.00	NIST Webbook
rinpol	1150.00	NIST Webbook
rinpol	1145.00	NIST Webbook
rinpol	1158.00	NIST Webbook
rinpol	1161.00	NIST Webbook
rinpol	1167.00	NIST Webbook
rinpol	1158.00	NIST Webbook
rinpol	1148.00	NIST Webbook
rinpol	1144.00	NIST Webbook
rinpol	1158.00	NIST Webbook
rinpol	1135.00	NIST Webbook
rinpol	1164.90	NIST Webbook
rinpol	1168.00	NIST Webbook
rinpol	1110.00	NIST Webbook
rinpol	1154.00	NIST Webbook
rinpol	1162.00	NIST Webbook
rinpol	1166.00	NIST Webbook
rinpol	1151.00	NIST Webbook
rinpol	1143.00	NIST Webbook
rinpol	1143.00	NIST Webbook
rinpol	1143.00	NIST Webbook
rinpol	1135.50	NIST Webbook
rinpol	1141.00	NIST Webbook
rinpol	1145.00	NIST Webbook
rinpol	1146.00	NIST Webbook
rinpol	1150.00	NIST Webbook
rinpol	1158.00	NIST Webbook
rinpol	1164.90	NIST Webbook
rinpol	1163.00	NIST Webbook
rinpol	1143.10	NIST Webbook
rinpol	1145.00	NIST Webbook
rinpol	1134.00	NIST Webbook
rinpol	1155.95	NIST Webbook
rinpol	1160.10	NIST Webbook
rinpol	1148.70	NIST Webbook
rinpol	1142.00	NIST Webbook

rinpol	1140.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1144.90		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1163.50		NIST Webbook
rinpol	1168.20		NIST Webbook
ripol	1470.20		NIST Webbook
ripol	1394.10		NIST Webbook
ripol	1376.30		NIST Webbook
ripol	1433.30		NIST Webbook
ripol	1409.00		NIST Webbook
ripol	1416.00		NIST Webbook
ripol	1408.00		NIST Webbook
ripol	1433.00		NIST Webbook
ripol	1414.00		NIST Webbook
ripol	1414.00		NIST Webbook
ripol	1426.00		NIST Webbook
ripol	1439.00		NIST Webbook
ripol	1453.00		NIST Webbook
ripol	1402.00		NIST Webbook
ripol	1376.00		NIST Webbook
ripol	1421.00		NIST Webbook
ripol	1422.00		NIST Webbook
ripol	1403.00		NIST Webbook
ripol	1419.00		NIST Webbook
ripol	1426.00		NIST Webbook
ripol	1426.00		NIST Webbook
ripol	1426.00		NIST Webbook
ripol	1376.00		NIST Webbook
ripol	1381.00		NIST Webbook
ripol	1426.00		NIST Webbook
ripol	1464.80		NIST Webbook
ripol	1459.30		NIST Webbook
ripol	1404.30		NIST Webbook
tb	478.60 ± 0.40	K	NIST Webbook
tb	468.00 ± 10.00	K	NIST Webbook
tb	461.00 ± 10.00	K	NIST Webbook
tb	478.60	K	KDB
tb	478.60	K	NIST Webbook
tb	478.35 ± 0.40	K	NIST Webbook

tb	461.00 ± 10.00	K	NIST Webbook
tb	452.00 ± 12.00	K	NIST Webbook
tb	477.40 ± 1.00	K	NIST Webbook
tb	478.00 ± 2.00	K	NIST Webbook
tb	478.00 ± 2.00	K	NIST Webbook
tb	478.00 ± 3.00	K	NIST Webbook
tb	478.00 ± 3.00	K	NIST Webbook
tb	471.70 ± 4.00	K	NIST Webbook
tb	478.50 ± 2.00	K	NIST Webbook
tb	473.00 ± 4.00	K	NIST Webbook
tb	473.15 ± 2.00	K	NIST Webbook
tb	473.15 ± 2.00	K	NIST Webbook
tb	475.00 ± 5.00	K	NIST Webbook
tb	475.10 ± 3.00	K	NIST Webbook
tb	470.00 ± 5.00	K	NIST Webbook
tb	453.00 ± 15.00	K	NIST Webbook
tb	461.00 ± 10.00	K	NIST Webbook
tc	679.90	K	KDB
tf	198.00	K	KDB
tf	194.90 ± 0.30	K	NIST Webbook
vc	0.550	m3/kmol	KDB
zc	0.2529610		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.96	J/mol×K	679.70	Joback Method
cpg	315.99	J/mol×K	511.42	Joback Method
cpg	331.19	J/mol×K	545.07	Joback Method
cpg	345.55	J/mol×K	578.73	Joback Method
cpg	359.11	J/mol×K	612.39	Joback Method
cpg	371.90	J/mol×K	646.04	Joback Method
cpg	299.93	J/mol×K	477.76	Joback Method
dvisc	0.0038056	Pa×s	240.15	Joback Method
dvisc	0.0016875	Pa×s	279.75	Joback Method
dvisc	0.0009155	Pa×s	319.35	Joback Method
dvisc	0.0005684	Pa×s	358.96	Joback Method
dvisc	0.0003880	Pa×s	398.56	Joback Method
dvisc	0.0002837	Pa×s	438.16	Joback Method
dvisc	0.0002186	Pa×s	477.76	Joback Method
hvapt	41.21	kJ/mol	478.60	KDB

pvap	0.22	kPa	320.30	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	0.02	kPa	284.50	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	0.18	kPa	317.30	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	0.15	kPa	314.20	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	0.12	kPa	311.20	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	0.10	kPa	308.20	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	0.09	kPa	306.30	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	0.07	kPa	303.20	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	0.05	kPa	298.30	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes

pvap	0.04	kPa	296.30	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	0.03	kPa	293.40	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	0.03	kPa	293.30	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	0.03	kPa	290.40	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	0.02	kPa	287.50	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
pvap	0.27	kPa	323.20	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes
rfi	1.48870		293.10	Extraction of pentylbenzene from high molar mass alkanes (C14 and C17) by N-methyl-2-pyrrolidone

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)

Coeff. A	1.48785e+01
Coeff. B	-4.46183e+03
Coeff. C	-4.37410e+01
Temperature range (K), min.	349.54
Temperature range (K), max.	510.12

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.28216e+01
Coeff. B	-8.15428e+03
Coeff. C	-6.76421e+00
Coeff. D	2.50375e-06
Temperature range (K), min.	198.15
Temperature range (K), max.	679.90

Sources

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	https://www.doi.org/10.1021/je050440b
Vapour pressures and enthalpies of vaporization of a series of the linear Trimethyl-butylammonium Bis(trifluoromethylsulfonyl) Imide	https://www.doi.org/10.1016/j.jct.2005.11.009
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
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	https://www.doi.org/10.1021/je0503554
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Paramagnetic Ionic Liquid 1-Butyl-3-methylimidazolium Bis(trifluoromethylsulfonyl) Imide	https://www.doi.org/10.1021/je800846j
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Activity Coefficients at Infinite Dilution of Organic Solutes and Crystal Structure:	https://www.doi.org/10.1016/j.jct.2008.09.004
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C538681&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Chromatography:	https://www.doi.org/10.1016/j.fluid.2006.07.015
Experimental Study of Thermodynamic Properties of Mixtures Containing Ionic Liquids and Toluene Using Gas-Liquid Chromatography and Transpiration Method:	https://www.doi.org/10.1021/je0602723
Extraction of pentylbenzene from high molar mass alkanes (C14 and C17) by 1-ethyl-2-pyrrolidone:	https://www.doi.org/10.1016/j.jct.2005.06.012
KDB:	https://www.cheric.org/files/research/kdb/mol/mol687.mol
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=687

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
rfi:	Refractive Index
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility