

# Benzene, hexyl-

<b>Other names:</b>	1-PHENYLHEXYLBENZENE 1-Phenylhexane Hexane, 1-phenyl- Hexylbenzene n-Hexylbenzene
<b>Inchi:</b>	InChI=1S/C12H18/c1-2-3-4-6-9-12-10-7-5-8-11-12/h5,7-8,10-11H,2-4,6,9H2,1H3
<b>InchiKey:</b>	LTEQMZWBSYACLV-UHFFFAOYSA-N
<b>Formula:</b>	C12H18
<b>SMILES:</b>	CCCCCc1ccccc1
<b>Mol. weight [g/mol]:</b>	162.27
<b>CAS:</b>	1077-16-3

## Physical Properties

Property code	Value	Unit	Source
af	0.4800		KDB
gf	162.57	kJ/mol	Joback Method
hf	-54.48	kJ/mol	Joback Method
hfus	20.88	kJ/mol	Joback Method
hvap	60.00	kJ/mol	NIST Webbook
hvap	60.20	kJ/mol	NIST Webbook
log10ws	-5.21		Aqueous Solubility Prediction Method
log10ws	-5.21		Estimated Solubility Method
logp	3.809		Crippen Method
mvol	156.180	ml/mol	McGowan Method
pc	2380.00	kPa	KDB
rinpol	1230.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1248.08		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1247.20		NIST Webbook
rinpol	1254.60		NIST Webbook
rinpol	213.10		NIST Webbook
rinpol	1245.00		NIST Webbook

rinpol	1244.00	NIST Webbook
rinpol	1267.20	NIST Webbook
rinpol	1242.00	NIST Webbook
rinpol	1254.00	NIST Webbook
rinpol	1262.00	NIST Webbook
rinpol	1220.00	NIST Webbook
rinpol	1256.00	NIST Webbook
rinpol	1244.00	NIST Webbook
rinpol	1246.00	NIST Webbook
rinpol	1244.00	NIST Webbook
rinpol	1266.48	NIST Webbook
rinpol	1263.43	NIST Webbook
rinpol	1259.18	NIST Webbook
rinpol	1256.00	NIST Webbook
rinpol	1248.08	NIST Webbook
rinpol	1256.20	NIST Webbook
rinpol	1245.30	NIST Webbook
rinpol	1241.23	NIST Webbook
rinpol	1247.00	NIST Webbook
rinpol	1254.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1260.90	NIST Webbook
rinpol	1258.40	NIST Webbook
rinpol	1254.60	NIST Webbook
rinpol	1247.30	NIST Webbook
rinpol	1247.20	NIST Webbook
rinpol	1245.20	NIST Webbook
rinpol	1233.00	NIST Webbook
rinpol	1260.90	NIST Webbook
rinpol	1258.40	NIST Webbook
rinpol	1256.00	NIST Webbook
rinpol	1254.60	NIST Webbook
rinpol	1252.75	NIST Webbook
rinpol	1244.00	NIST Webbook
rinpol	1259.00	NIST Webbook
rinpol	1235.00	NIST Webbook
rinpol	1255.00	NIST Webbook
rinpol	1239.00	NIST Webbook
rinpol	1260.00	NIST Webbook
rinpol	1271.00	NIST Webbook
rinpol	1244.00	NIST Webbook
rinpol	1230.00	NIST Webbook
rinpol	1264.00	NIST Webbook
rinpol	1263.00	NIST Webbook

rinpol	1244.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1239.70		NIST Webbook
rinpol	1225.40		NIST Webbook
rinpol	1228.80		NIST Webbook
rinpol	1243.60		NIST Webbook
rinpol	1249.70		NIST Webbook
rinpol	1256.20		NIST Webbook
rinpol	1225.40		NIST Webbook
rinpol	1228.80		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1259.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1231.20		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1228.00		NIST Webbook
ripol	1551.00		NIST Webbook
ripol	1531.00		NIST Webbook
ripol	1532.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1537.00		NIST Webbook
ripol	1524.00		NIST Webbook
ripol	1513.00		NIST Webbook
ripol	1513.00		NIST Webbook
ripol	1515.00		NIST Webbook
ripol	1499.00		NIST Webbook
ripol	1529.00		NIST Webbook
ripol	1531.00		NIST Webbook
ripol	1489.20		NIST Webbook
ripol	1578.90		NIST Webbook
ripol	1573.20		NIST Webbook
ripol	1567.50		NIST Webbook
ripol	1561.80		NIST Webbook
ripol	1556.10		NIST Webbook
tb	500.00 ± 4.00	K	NIST Webbook
tb	499.30	K	KDB
tb	481.00 ± 6.00	K	NIST Webbook
tb	493.00 ± 5.00	K	NIST Webbook
tb	488.00 ± 5.00	K	NIST Webbook
tb	488.15 ± 2.00	K	NIST Webbook

tb	500.50 ± 1.00	K	NIST Webbook
tb	494.00 ± 6.00	K	NIST Webbook
tb	492.00 ± 5.00	K	NIST Webbook
tb	492.00 ± 5.00	K	NIST Webbook
tb	499.00 ± 6.00	K	NIST Webbook
tb	500.00 ± 5.00	K	NIST Webbook
tb	499.30	K	NIST Webbook
tb	500.00 ± 4.00	K	NIST Webbook
tb	494.00 ± 3.00	K	NIST Webbook
tb	487.00 ± 20.00	K	NIST Webbook
tb	485.00 ± 6.00	K	NIST Webbook
tb	491.00 ± 12.00	K	NIST Webbook
tb	490.00 ± 10.00	K	NIST Webbook
tb	498.15 ± 1.50	K	NIST Webbook
tb	488.65 ± 1.50	K	NIST Webbook
tb	498.92 ± 0.50	K	NIST Webbook
tb	498.92 ± 0.20	K	NIST Webbook
tb	498.90 ± 0.50	K	NIST Webbook
tc	697.50	K	KDB
tf	206.40 ± 1.50	K	NIST Webbook
tf	209.70 ± 0.50	K	NIST Webbook
tf	209.70 ± 0.30	K	NIST Webbook
tf	212.00	K	KDB
vc	0.620	m <sup>3</sup> /kmol	KDB
zc	0.2544410		KDB

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.87	J/mol×K	699.90	Joback Method
cpg	362.33	J/mol×K	533.85	Joback Method
cpg	378.30	J/mol×K	567.06	Joback Method
cpg	393.41	J/mol×K	600.27	Joback Method
cpg	407.68	J/mol×K	633.48	Joback Method
cpg	421.16	J/mol×K	666.69	Joback Method
cpg	345.46	J/mol×K	500.64	Joback Method
cpl	248.00	J/mol×K	293.00	NIST Webbook
dvisc	0.0002707	Paxs	459.10	Joback Method
dvisc	0.0003725	Paxs	417.57	Joback Method
dvisc	0.0005501	Paxs	376.03	Joback Method
dvisc	0.0008950	Paxs	334.49	Joback Method

dvisc	0.0016716	Paxs	292.96	Joback Method
dvisc	0.0002074	Paxs	500.64	Joback Method
dvisc	0.0038377	Paxs	251.42	Joback Method
hvapt	43.09	kJ/mol	499.30	KDB
hvapt	61.60	kJ/mol	368.50	NIST Webbook
rho1	819.50	kg/m3	343.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Selected Ternary Mixtures of n-Butylcyclohexane + a Linear Alkane (n-Hexadecane or n-Dodecane) + an Aromatic Compound (Toluene, n-Butylbenzene, or n-Hexylbenzene)
rho1	851.00	kg/m3	303.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of n-Hexylbenzene (1) or n-Butylbenzene (1) in 2,2,4,6,6-Pentamethylheptane (2) or 2,2,4,4,6,8,8-Heptamethylnonane (2) at 0.1 MPa
rho1	843.40	kg/m3	313.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of n-Hexylbenzene (1) or n-Butylbenzene (1) in 2,2,4,6,6-Pentamethylheptane (2) or 2,2,4,4,6,8,8-Heptamethylnonane (2) at 0.1 MPa

rho1	835.80	kg/m3	323.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of n-Hexylbenzene (1) or n-Butylbenzene (1) in 2,2,4,6,6-Pentamethylheptane (2) or 2,2,4,4,6,8,8-Heptamethylnonane (2) at 0.1 MPa
rho1	828.20	kg/m3	333.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of n-Hexylbenzene (1) or n-Butylbenzene (1) in 2,2,4,6,6-Pentamethylheptane (2) or 2,2,4,4,6,8,8-Heptamethylnonane (2) at 0.1 MPa
rho1	858.60	kg/m3	293.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of n-Hexylbenzene (1) or n-Butylbenzene (1) in 2,2,4,6,6-Pentamethylheptane (2) or 2,2,4,4,6,8,8-Heptamethylnonane (2) at 0.1 MPa

rho1	827.48	kg/m3	333.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Selected Ternary Mixtures of n-Butylcyclohexane + a Linear Alkane (n-Hexadecane or n-Dodecane) + an Aromatic Compound (Toluene, n-Butylbenzene, or n-Hexylbenzene)
rho1	834.87	kg/m3	323.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Selected Ternary Mixtures of n-Butylcyclohexane + a Linear Alkane (n-Hexadecane or n-Dodecane) + an Aromatic Compound (Toluene, n-Butylbenzene, or n-Hexylbenzene)
rho1	842.49	kg/m3	313.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Selected Ternary Mixtures of n-Butylcyclohexane + a Linear Alkane (n-Hexadecane or n-Dodecane) + an Aromatic Compound (Toluene, n-Butylbenzene, or n-Hexylbenzene)

rhoI	850.09	kg/m3	303.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Selected Ternary Mixtures of n-Butylcyclohexane + a Linear Alkane (n-Hexadecane or n-Dodecane) + an Aromatic Compound (Toluene, n-Butylbenzene, or n-Hexylbenzene)
rhoI	857.69	kg/m3	293.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Selected Ternary Mixtures of n-Butylcyclohexane + a Linear Alkane (n-Hexadecane or n-Dodecane) + an Aromatic Compound (Toluene, n-Butylbenzene, or n-Hexylbenzene)
rhoI	862.40	kg/m3	288.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of n-Hexylbenzene (1) or n-Butylbenzene (1) in 2,2,4,6,6-Pentamethylheptane (2) or 2,2,4,4,6,8,8-Heptamethylnonane (2) at 0.1 MPa



rho1	889.10	kg/m3	253.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of n-Hexylbenzene (1) or n-Butylbenzene (1) in 2,2,4,6,6-Pentamethylheptane (2) or 2,2,4,4,6,8,8-Heptamethylnonane (2) at 0.1 MPa
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srf	0.03	N/m	294.40	Densities and Viscosities at 293.15 373.15 K, Speeds of Sound and Bulk Moduli at 293.15 333.15 K, Surface Tensions, and Flash Points of Binary Mixtures of n-Hexadecane and Alkylbenzenes at 0.1 MPa
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## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47833e+01
Coeff. B	-4.48545e+03
Coeff. C	-5.79950e+01
Temperature range (K), min.	367.43
Temperature range (K), max.	531.55

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	9.17344e+01
Coeff. B	-1.01347e+04
Coeff. C	-1.09214e+01
Coeff. D	4.18024e-06
Temperature range (K), min.	212.00

## Sources

- Densities and Viscosities of Ternary Mixtures of Heptane, Octane, Nonane, and Decane with Benzene from 293.15 K to 310.15 K + Hexylbenzene + Sulfolane: Joback Method: <https://www.doi.org/10.1021/je700202h>
- Crippen Method: <https://www.doi.org/10.1021/je7000123>
- Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and KDB Point of Selected Ternary Mixtures of n-Butylcyclohexane + a Linear Alkane (n-Hexadecane or 1-Pentadecane), Air, and Liquid Dumbbells: [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)
- Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and KDB Point of Selected Ternary Mixtures of n-Butylcyclohexane + a Linear Alkane (n-Hexadecane or 1-Pentadecane), Air, and Liquid Dumbbells: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
- Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and KDB Point of Selected Ternary Mixtures of n-Butylcyclohexane + a Linear Alkane (n-Hexadecane or 1-Pentadecane), Air, and Liquid Dumbbells: <https://www.doi.org/10.1021/acs.jced.7b00466>
- Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and KDB Point of Selected Ternary Mixtures of n-Butylcyclohexane + a Linear Alkane (n-Hexadecane or 1-Pentadecane), Air, and Liquid Dumbbells: <https://www.thermo.com/files/research/kdb/mol/mol698.mol>
- Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and KDB Point of Selected Ternary Mixtures of n-Butylcyclohexane + a Linear Alkane (n-Hexadecane or 1-Pentadecane), Air, and Liquid Dumbbells: <https://www.doi.org/10.1021/acs.jced.7b00087>
- Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and KDB Point of Selected Ternary Mixtures of n-Butylcyclohexane + a Linear Alkane (n-Hexadecane or 1-Pentadecane), Air, and Liquid Dumbbells: <https://www.doi.org/10.1021/je050273f>
- Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and KDB Point of Selected Ternary Mixtures of n-Butylcyclohexane + a Linear Alkane (n-Hexadecane or 1-Pentadecane), Air, and Liquid Dumbbells: <https://www.doi.org/10.1016/j.fluid.2005.09.021>
- The Yaws Handbook of Vapor Pressure: KDB Vapor Pressure Data: [http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl\\_file/ci034243xsi20040112\\_053635.txt](http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt)
- Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and KDB Point of Binary Mixtures of n-Hexylbenzene (1) or n-Butylbenzene (1) in 2,2,4,6,6-Pentamethylheptane (2) or 2,2,4,4,6,8,8-Heptamethylnonane (2) at Infinite Dilution: <https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
- Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and KDB Point of Binary Mixtures of n-Hexylbenzene (1) or n-Butylbenzene (1) in 2,2,4,6,6-Pentamethylheptane (2) or 2,2,4,4,6,8,8-Heptamethylnonane (2) at Infinite Dilution: <https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=698>
- Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and KDB Point of Binary Mixtures of n-Hexylbenzene (1) or n-Butylbenzene (1) in 2,2,4,6,6-Pentamethylheptane (2) or 2,2,4,4,6,8,8-Heptamethylnonane (2) at Infinite Dilution: <https://www.doi.org/10.1021/acs.jced.8b00387>
- Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and KDB Point of Binary Mixtures of n-Hexylbenzene (1) or n-Butylbenzene (1) in 2,2,4,6,6-Pentamethylheptane (2) or 2,2,4,4,6,8,8-Heptamethylnonane (2) at Infinite Dilution: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1077163&Units=SI>
- Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and KDB Point of Binary Mixtures of n-Hexylbenzene (1) or n-Butylbenzene (1) in 2,2,4,6,6-Pentamethylheptane (2) or 2,2,4,4,6,8,8-Heptamethylnonane (2) at Infinite Dilution: <http://link.springer.com/article/10.1007/BF02311772>
- Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and KDB Point of Binary Mixtures of n-Hexylbenzene (1) or n-Butylbenzene (1) in 2,2,4,6,6-Pentamethylheptane (2) or 2,2,4,4,6,8,8-Heptamethylnonane (2) at Infinite Dilution: <https://www.doi.org/10.1016/j.fluid.2006.07.015>
- Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and KDB Point of Binary Mixtures of n-Hexylbenzene (1) or n-Butylbenzene (1) in 2,2,4,6,6-Pentamethylheptane (2) or 2,2,4,4,6,8,8-Heptamethylnonane (2) at Infinite Dilution: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

## 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
- 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

<b>rho:</b>	Liquid Density
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>srf:</b>	Surface Tension
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume
<b>zc:</b>	Critical Compressibility

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