Benzene, tert-butyl-

Other names:	(1,1-dimethylethyl)benzene 1,1-Dimethylethyl-benzene 2-METHYL-2-PHENYLPROPANE 2-PHENYL-2-METHYLPROPANE Benzene, (1,1-dimethylethyl)- Benzene, t-butyl- DIMETHYLETHYLBENZENE NSC 6557 Phenyltrimethylmethane Pseudobutylbenzene Trimethylphenylmethane benzene, 1,1-dimethylethyl- t-Butylbenzene tert-Butylbenzene «alpha»-dimethylethylbenzene Â«alphaÂ»-dimethylethylbenzene
Inchi:	InChI=1S/C10H14/c1-10(2,3)9-7-5-4-6-8-9/h4-8H,1-3H3
InchiKey:	YTZKOQUCBOVLHL-UHFFFAOYSA-N
Formula:	C10H14
SMILES:	CC(C)(C)c1ccccc1
Mol. weight [g/mol]:	134.22
CAS:	98-06-6

Physical Properties

Property code	Value	Unit	Source
af	0.2650		KDB
chl	-5865.20 ± 1.10	kJ/mol	NIST Webbook
chl	-5856.76	kJ/mol	NIST Webbook
chl	-5859.60	kJ/mol	NIST Webbook
dm	0.50	debye	KDB
gf	148.57	kJ/mol	Joback Method
hcg	5867.22	kJ/mol	KDB
hcn	5559.700	kJ/mol	KDB
hf	-22.69	kJ/mol	KDB
hf	-22.70 ± 1.40	kJ/mol	NIST Webbook
hfl	-70.80 ± 1.30	kJ/mol	NIST Webbook

hfus	8.39	kJ/mol	Thermodynamic properties of tert-butylbenzene and 1,4-di-tert-butylbenzene
hvap	38.83	kJ/mol	Joback Method
ie	8.65	eV	NIST Webbook
ie	8.25	eV	NIST Webbook
ie	8.63 ± 0.01	eV	NIST Webbook
ie	8.68 ± 0.03	eV	NIST Webbook
ie	8.69	eV	NIST Webbook
ie	8.74 ± 0.05	eV	NIST Webbook
ie	8.72 ± 0.01	eV	NIST Webbook
ie	8.64	eV	NIST Webbook
ie	8.68 ± 0.01	eV	NIST Webbook
ie	8.68 ± 0.01	eV	NIST Webbook
ie	8.83	eV	NIST Webbook
ie	8.81	eV	NIST Webbook
ie	8.69	eV	NIST Webbook
log10ws	-3.66		Estimated Solubility Method
log10ws	-3.66		Aqueous Solubility Prediction Method
logp	2.984		Crippen Method
mcvol	128.000	ml/mol	McGowan Method
pc	2960.00	kPa	KDB
rinpol	986.90		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	992.50		NIST Webbook
rinpol	980.90		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	974.00		NIST Webbook
rinpol	971.00		NIST Webbook
rinpol	974.90		NIST Webbook
rinpol	975.40		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	988.00		NIST Webbook

rinpol	994.00	NIST Webbook
rinpol	1001.00	NIST Webbook
rinpol	969.90	NIST Webbook
rinpol	972.50	NIST Webbook
rinpol	987.60	NIST Webbook
rinpol	993.50	NIST Webbook
rinpol	1000.90	NIST Webbook
rinpol	975.00	NIST Webbook
rinpol	969.90	NIST Webbook
rinpol	969.90	NIST Webbook
rinpol	972.50	NIST Webbook
rinpol	972.00	NIST Webbook
rinpol	967.08	NIST Webbook
rinpol	975.40	NIST Webbook
rinpol	973.30	NIST Webbook
rinpol	976.00	NIST Webbook
rinpol	992.00	NIST Webbook
rinpol	985.00	NIST Webbook
rinpol	981.00	NIST Webbook
rinpol	988.00	NIST Webbook
rinpol	987.10	NIST Webbook
rinpol	990.50	NIST Webbook
rinpol	992.00	NIST Webbook
rinpol	972.40	NIST Webbook
rinpol	979.30	NIST Webbook
rinpol	979.10	NIST Webbook
rinpol	987.10	NIST Webbook
rinpol	990.50	NIST Webbook
rinpol	992.00	NIST Webbook
rinpol	978.00	NIST Webbook
rinpol	988.00	NIST Webbook
rinpol	972.82	NIST Webbook
rinpol	976.53	NIST Webbook
rinpol	978.96	NIST Webbook
rinpol	989.31	NIST Webbook
rinpol	993.20	NIST Webbook
rinpol	995.68	NIST Webbook
rinpol	976.00	NIST Webbook
rinpol	1001.00	NIST Webbook
rinpol	988.00	NIST Webbook
rinpol	963.00	NIST Webbook
rinpol	976.00	NIST Webbook
rinpol	994.00	NIST Webbook
rinpol	977.00	NIST Webbook

rinpol	984.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	971.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	971.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	973.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	986.40		NIST Webbook
rinpol	993.80		NIST Webbook
rinpol	991.70		NIST Webbook
rinpol	991.90		NIST Webbook
rinpol	973.30		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	983.22		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	961.00		NIST Webbook
ripol	1249.00		NIST Webbook
ripol	1237.50		NIST Webbook
ripol	1229.50		NIST Webbook
ripol	1215.10		NIST Webbook
ripol	1223.00		NIST Webbook
ripol	1247.00		NIST Webbook
ripol	1215.00		NIST Webbook
ripol	1239.00		NIST Webbook
ripol	1229.00		NIST Webbook
ripol	1287.00		NIST Webbook
ripol	1275.00		NIST Webbook
ripol	1262.00		NIST Webbook
ripol	1251.00		NIST Webbook
ripol	1215.00		NIST Webbook
sl	278.70	J/mol×K	NIST Webbook
tb	442.30	K	KDB
tc	660.00	K	KDB
tf	214.82	K	Aqueous Solubility Prediction Method
tf	215.30	K	KDB
tt	215.00 ± 0.20	K	NIST Webbook
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.46	J/mol×K	633.88	Joback Method
cpg	258.79	J/mol×K	451.65	Joback Method
cpg	275.46	J/mol×K	488.10	Joback Method
cpg	290.99	J/mol×K	524.54	Joback Method
cpg	305.47	J/mol×K	560.99	Joback Method
cpg	318.94	J/mol×K	597.44	Joback Method
cpg	343.10	J/mol×K	670.33	Joback Method
cpl	238.11	J/mol×K	294.30	NIST Webbook
dvisc	0.0002313	Pa×s	451.65	Joback Method
dvisc	0.0057820	Pa×s	231.30	Joback Method
dvisc	0.0023414	Pa×s	268.02	Joback Method
dvisc	0.0011790	Pa×s	304.75	Joback Method
dvisc	0.0006880	Pa×s	341.48	Joback Method
dvisc	0.0004458	Pa×s	378.20	Joback Method
dvisc	0.0003119	Pa×s	414.92	Joback Method
hfust	8.40	kJ/mol	215.00	NIST Webbook
hfust	8.40	kJ/mol	215.30	NIST Webbook
hfust	8.41	kJ/mol	215.00	NIST Webbook
hfust	8.40	kJ/mol	215.00	NIST Webbook
hvapt	43.10	kJ/mol	406.00	NIST Webbook
hvapt	45.30 ± 0.20	kJ/mol	409.00	NIST Webbook
hvapt	43.70	kJ/mol	400.00	NIST Webbook
hvapt	39.90 ± 0.30	kJ/mol	409.00	NIST Webbook
hvapt	37.00 ± 0.50	kJ/mol	409.00	NIST Webbook
hvapt	47.80 ± 0.40	kJ/mol	293.00	NIST Webbook
hvapt	42.60 ± 0.20	kJ/mol	409.00	NIST Webbook
rfi	1.48007		318.15	Volumetric and refractive properties of 1,3,5,7-tetravinyl-1,3,5,7-tetramethylcyclotetrasiloxane with methoxybenzene, chlorobenzene, tert-butylbenzene and nitrobenzene at T = (298.15-318.15) K
rfi	1.49024		298.15	KDB

rfi	1.49003	298.15	Effect of Temperature on the Change of Refractive Index on Mixing for Butyl Acetate + Aromatic Hydrocarbons
rfi	1.49009	298.15	Volumetric and refractive properties of 1,3,5,7-tetravinyl-1,3,5,7-tetramethylcyclotetrasiloxane with methoxybenzene, chlorobenzene, tert-butylbenzene and nitrobenzene at T = (298.15-318.15) K
rfi	1.49018	298.15	Volumetric and refractive properties of 1,3,5,7-tetravinyl-1,3,5,7-tetramethylcyclotetrasiloxane with methoxybenzene, chlorobenzene, tert-butylbenzene and nitrobenzene at T = (298.15-318.15) K
rfi	1.48763	303.15	Volumetric and refractive properties of 1,3,5,7-tetravinyl-1,3,5,7-tetramethylcyclotetrasiloxane with methoxybenzene, chlorobenzene, tert-butylbenzene and nitrobenzene at T = (298.15-318.15) K
rfi	1.48509	308.15	Volumetric and refractive properties of 1,3,5,7-tetravinyl-1,3,5,7-tetramethylcyclotetrasiloxane with methoxybenzene, chlorobenzene, tert-butylbenzene and nitrobenzene at T = (298.15-318.15) K

rfi	1.48256		313.15	Volumetric and refractive properties of 1,3,5,7-tetravinyl-1,3,5,7-tetramethylcyclotetrasiloxane with methoxybenzene, chlorobenzene, tert-butylbenzene and nitrobenzene at T = (298.15-318.15) K
rhol	862.23	kg/m3	298.15	Thermodynamic study of 1,1,2,2-tetrachloroethane + hydrocarbon mixtures I. Excess and solvation enthalpies
rhol	867.00	kg/m3	293.00	KDB
rhol	862.28	kg/m3	298.15	The physicochemical properties of 1,3,5-trimethyl-1,3,5-tris(3,3,3-trifluoropropyl)cyclotrisiloxane with various aromatic hydrocarbons at T = (308.15 to 323.15) K
rhol	854.12	kg/m3	308.15	The physicochemical properties of 1,3,5-trimethyl-1,3,5-tris(3,3,3-trifluoropropyl)cyclotrisiloxane with various aromatic hydrocarbons at T = (308.15 to 323.15) K
rhol	849.98	kg/m3	313.15	The physicochemical properties of 1,3,5-trimethyl-1,3,5-tris(3,3,3-trifluoropropyl)cyclotrisiloxane with various aromatic hydrocarbons at T = (308.15 to 323.15) K
rhol	845.87	kg/m3	318.15	The physicochemical properties of 1,3,5-trimethyl-1,3,5-tris(3,3,3-trifluoropropyl)cyclotrisiloxane with various aromatic hydrocarbons at T = (308.15 to 323.15) K

rhol	841.72	kg/m3	323.15	The physicochemical properties of 1,3,5-trimethyl-1,3,5-tris(3,3,3-trifluoropropyl)cyclotrisiloxane with various aromatic hydrocarbons at T = (308.15 to 323.15) K
sfust	39.06	J/mol×K	215.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38431e+01
Coeff. B	-3.47592e+03
Coeff. C	-6.54960e+01
Temperature range (K), min.	321.92
Temperature range (K), max.	472.91

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.26802e+01
Coeff. B	-8.94559e+03
Coeff. C	-1.13016e+01
Coeff. D	5.13608e-06
Temperature range (K), min.	215.27
Temperature range (K), max.	660.00

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
298.15	100.00	862.38

313.15	100.00	849.98
333.15	100.00	833.32
353.15	100.00	816.42
373.15	100.00	799.33
393.15	100.00	781.81
413.15	100.00	763.74
433.15	100.00	745.23
298.15	20100.00	875.86
313.15	20100.00	864.52
333.15	20100.00	849.54
353.15	20100.00	834.5
373.15	20100.00	819.57
393.15	20100.00	804.5
413.15	20100.00	789.38
433.15	20100.00	774.28
298.15	40100.00	887.54
313.15	40100.00	877.0
333.15	40100.00	863.16
353.15	40100.00	849.4
373.15	40100.00	835.86
393.15	40100.00	822.33
413.15	40100.00	808.84
433.15	40100.00	795.55
298.15	60100.00	897.94
313.15	60100.00	888.01
333.15	60100.00	875.06
353.15	60100.00	862.22
373.15	60100.00	849.64
393.15	60100.00	837.18
413.15	60100.00	824.82
433.15	60100.00	812.75
298.15	80100.00	907.35
313.15	80100.00	897.93
333.15	80100.00	885.65
353.15	80100.00	873.52
373.15	80100.00	861.72
393.15	80100.00	850.05
413.15	80100.00	838.52
433.15	80100.00	827.29
298.15	100100.00	915.98
313.15	100100.00	906.96
333.15	100100.00	895.25
353.15	100100.00	883.72
373.15	100100.00	872.52

393.15	100100.00	861.47
413.15	100100.00	850.58
433.15	100100.00	840.05

Reference *https://www.doi.org/10.1016/j.fluid.2018.02.008*

Speed of sound, m/s

Temperature, K - Liquid	Pressure, kPa - Liquid	Speed of sound, m/s - Liquid
298.15	100.00	1316.4
313.15	100.00	1255.3
333.15	100.00	1176.9
353.15	100.00	1101.8
373.15	100.00	1029.9
393.15	100.00	959.3
413.15	100.00	890.9
433.15	100.00	823.7
298.15	20100.00	1415.8
313.15	20100.00	1360.3
333.15	20100.00	1290.1
353.15	20100.00	1223.5
373.15	20100.00	1161.2
393.15	20100.00	1101.1
413.15	20100.00	1042.6
433.15	20100.00	987.2
298.15	40100.00	1501.7
313.15	40100.00	1450.3
333.15	40100.00	1385.4
353.15	40100.00	1324.4
373.15	40100.00	1267.7
393.15	40100.00	1213.3
413.15	40100.00	1161.1
433.15	40100.00	1112.1
298.15	60100.00	1578.5
313.15	60100.00	1529.8
333.15	60100.00	1469.0
353.15	60100.00	1411.8
373.15	60100.00	1359.0
393.15	60100.00	1308.5
413.15	60100.00	1260.2
433.15	60100.00	1215.1

298.15	80100.00	1647.9
313.15	80100.00	1601.7
333.15	80100.00	1543.9
353.15	80100.00	1489.6
373.15	80100.00	1439.6
393.15	80100.00	1392.0
413.15	80100.00	1346.6
433.15	80100.00	1304.3
298.15	100100.00	1711.7
313.15	100100.00	1667.3
333.15	100100.00	1612.5
353.15	100100.00	1560.2
373.15	100100.00	1512.4
393.15	100100.00	1466.9
413.15	100100.00	1423.8
433.15	100100.00	1383.6

Reference *https://www.doi.org/10.1016/j.jct.2019.03.005*

Sources

Thermodynamic properties of cumene, tert-butylbenzene, and n-hexadecane under elevated pressures: https://www.doi.org/10.1016/j.jct.2019.03.005

Effect of Temperature on the Change of Refractive Index on Mixing for Butyl Acetate + Aromatic Hydrocarbons: https://www.doi.org/10.1007/s10765-005-8096-3

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

The physicochemical properties of 1,3,5-trimethyl-1,3,5-tris(3,3,3-trifluoropropyl)cyclotrisiloxane with various aromatic hydrocarbons at T = (308.15 to 323.15) K: https://www.doi.org/10.1016/j.jct.2015.12.025

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=668

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C98066&Units=SI

Thermodynamic properties of tert-butylbenzene and 1,4-di-tert-butylbenzene: https://www.doi.org/10.1016/j.jct.2008.10.008

Volumetric and refractive properties of 1,3,5,7-tetravinyl-1,3,5,7-tetramethylcyclotetrasiloxane with methoxybenzene, chlorobenzene, tert-butylbenzene and nitrobenzene at T = (298.15-318.15) K: https://www.doi.org/10.1016/j.jct.2018.09.021

Thermochemistry of ionic liquid catalysed reactions: https://www.doi.org/10.1016/j.jct.2010.01.006

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Transferability of tert-alkyl-benzenes. Are these systems ideal?: https://www.doi.org/10.1016/j.fluid.2006.10.013

Thermodynamic study of 1,1,2,2-tetrachloroethane + hydrocarbon mixtures I. Excess and solution enthalpies: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

The Yaws Handbook of Vapor Pressure:

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Determination of Henry's Law Constants Using Internal Standards With Benchmark Values: https://www.doi.org/10.1021/je3010535

KDB: https://www.cheric.org/files/research/kdb/mol/mol668.mol

Saturated Heat Capacities of Some Linear and Branched Alkylbenzenes between (332 and 481) K: https://www.doi.org/10.1021/je050273f

Liquid density measurements of cumene, tert-butylbenzene, and hexadecane over wide ranges of temperature and pressure: https://www.doi.org/10.1016/j.fluid.2018.02.008

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hcg:	Heat of Combustion, Gross form
hcn:	Heat of Combustion, Net Form
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
ie:	Ionization energy
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
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
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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