Benzene, (1-methylpropyl)-

Other names:	(1-Methylpropyl)benzene
	1-METHYL-PROPYLBENZENE
	2-PHENYLBUTANE
	Benzene, sec-butyl-
	SEC-BUTYLBENZENE
	Secondary butylbenzene
	UN 2709
	s-Butylbenzene
	«alpha»-methylpropylbenzene
	Â«alphaÂ»-methylpropylbenzene
Inchi:	InChI=1S/C10H14/c1-3-9(2)10-7-5-4-6-8-10/h4-9H,3H2,1-2H3
InchiKey:	ZJMWRROPUADPEA-UHFFFAOYSA-N
Formula:	C10H14
SMILES:	CCC(C)c1ccccc1
Mol. weight [g/mol]:	134.22
CAS:	135-98-8

Physical Properties

Property code	Value	Unit	Source
af	0.2740		KDB
chl	-5869.50 ± 1.10	kJ/mol	NIST Webbook
dm	0.40	debye	KDB
gf	143.29	kJ/mol	Joback Method
hcg	5877.68	kJ/mol	KDB
hcn	5570.160	kJ/mol	KDB
hf	-17.46	kJ/mol	KDB
hf	-17.40 ± 1.40	kJ/mol	NIST Webbook
hfl	-66.00 ± 1.00	kJ/mol	NIST Webbook
hfus	12.17	kJ/mol	Joback Method
hvap	48.60	kJ/mol	NIST Webbook
hvap	47.99	kJ/mol	NIST Webbook
hvap	48.10	kJ/mol	NIST Webbook
hvap	49.50	kJ/mol	NIST Webbook
ie	8.68 ± 0.01	eV	NIST Webbook
ie	8.68	eV	NIST Webbook
ie	8.68 ± 0.01	eV	NIST Webbook
ie	8.68 ± 0.01	eV	NIST Webbook

ie	8.66 ± 0.05	eV	NIST Webbook
log10ws	-3.08		Crippen Method
logp	3.200		Crippen Method
mcvol	128.000	ml/mol	McGowan Method
pc	2940.00	kPa	KDB
rinpol	997.00		NIST Webbook
rinpol	998.00		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	1011.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	1012.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	1015.20		NIST Webbook
rinpol	1008.70		NIST Webbook
rinpol	1010.70		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	998.00		NIST Webbook
rinpol	1004.90		NIST Webbook
rinpol	1010.90		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	987.00		NIST Webbook

rinpol	992.80	NIST Webbook
rinpol	993.30	NIST Webbook
rinpol	997.00	NIST Webbook
rinpol	1017.00	NIST Webbook
rinpol	1000.00	NIST Webbook
rinpol	1006.00	NIST Webbook
rinpol	1012.00	NIST Webbook
rinpol	1019.00	NIST Webbook
rinpol	997.00	NIST Webbook
rinpol	989.10	NIST Webbook
rinpol	1005.70	NIST Webbook
rinpol	1011.90	NIST Webbook
rinpol	1019.20	NIST Webbook
rinpol	986.40	NIST Webbook
rinpol	986.40	NIST Webbook
rinpol	989.10	NIST Webbook
rinpol	990.00	NIST Webbook
rinpol	983.15	NIST Webbook
rinpol	1015.00	NIST Webbook
rinpol	993.10	NIST Webbook
rinpol	993.10	NIST Webbook
rinpol	989.80	NIST Webbook
rinpol	995.00	NIST Webbook
rinpol	1010.00	NIST Webbook
rinpol	997.90	NIST Webbook
rinpol	995.00	NIST Webbook
rinpol	1014.00	NIST Webbook
rinpol	1006.40	NIST Webbook
rinpol	1008.90	NIST Webbook
rinpol	1011.70	NIST Webbook
rinpol	992.10	NIST Webbook
rinpol	994.10	NIST Webbook
rinpol	994.70	NIST Webbook
rinpol	999.10	NIST Webbook
rinpol	1006.40	NIST Webbook
rinpol	1008.90	NIST Webbook
rinpol	1011.70	NIST Webbook
rinpol	996.50	NIST Webbook
rinpol	996.78	NIST Webbook
rinpol	997.00	NIST Webbook
rinpol	1006.00	NIST Webbook
rinpol	995.00	NIST Webbook
rinpol	983.00	NIST Webbook
rinpol	994.00	NIST Webbook

rinpol	998.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	986.40		NIST Webbook
rinpol	996.00		NIST Webbook
ripol	1227.20		NIST Webbook
ripol	1248.10		NIST Webbook
ripol	1241.70		NIST Webbook
ripol	1248.00		NIST Webbook
ripol	1235.00		NIST Webbook
ripol	1248.00		NIST Webbook
ripol	1227.00		NIST Webbook
ripol	1248.00		NIST Webbook
ripol	1224.00		NIST Webbook
ripol	1311.00		NIST Webbook
ripol	1227.00		NIST Webbook
ripol	1250.00		NIST Webbook
ripol	1298.00		NIST Webbook
ripol	1287.00		NIST Webbook
ripol	1273.00		NIST Webbook
ripol	1260.00		NIST Webbook
ripol	1312.00		NIST Webbook
ripol	1259.00		NIST Webbook
ripol	1262.00		NIST Webbook
tb	446.50	K	KDB
tc	664.00	K	KDB
tf	197.70	K	KDB
tf	197.46 ± 0.10	K	NIST Webbook
tf	197.68 ± 0.04	K	NIST Webbook
tf	199.76 ± 0.20	K	NIST Webbook
tf	197.85 ± 0.20	K	NIST Webbook
tf	197.00 ± 0.70	K	NIST Webbook
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.43	J/mol×K	454.44	Joback Method
cpg	337.41	J/mol×K	663.87	Joback Method
cpg	325.87	J/mol×K	628.97	Joback Method

cpg	313.60	J/mol×K	594.06	Joback Method
cpg	300.56	J/mol×K	559.16	Joback Method
cpg	286.70	J/mol×K	524.25	Joback Method
cpg	272.00	J/mol×K	489.35	Joback Method
cpl	241.70	J/mol×K	293.74	NIST Webbook
dvisc	0.0021545	Pa×s	253.97	Joback Method
dvisc	0.0010588	Pa×s	294.07	Joback Method
dvisc	0.0006171	Pa×s	334.16	Joback Method
dvisc	0.0004037	Pa×s	374.25	Joback Method
dvisc	0.0002868	Pa×s	414.35	Joback Method
dvisc	0.0002163	Pa×s	454.44	Joback Method
dvisc	0.0057217	Pa×s	213.88	Joback Method
hvapt	43.20 ± 0.20	kJ/mol	413.00	NIST Webbook
hvapt	40.60 ± 0.30	kJ/mol	413.00	NIST Webbook
hvapt	37.80 ± 0.50	kJ/mol	413.00	NIST Webbook
hvapt	50.60	kJ/mol	308.00	NIST Webbook
hvapt	42.80	kJ/mol	416.00	NIST Webbook
hvapt	44.00	kJ/mol	408.00	NIST Webbook
hvapt	45.70 ± 0.20	kJ/mol	413.00	NIST Webbook
rfi	1.48779		298.15	KDB
rfi	1.48900		293.10	Phase equilibria for the extraction of sec-butylbenzene from dodecane with N,N-dimethylformamide
rhol	837.48	kg/m3	323.15	Densities, speeds of sound, refractive indices, viscosities and their related thermodynamic properties for n-hexadecane + two aromatic hydrocarbons binary mixtures at temperatures from 298.15 K to 318.15 K
rhol	861.95	kg/m3	293.15	Densities, speeds of sound, refractive indices, viscosities and their related thermodynamic properties for n-hexadecane + two aromatic hydrocarbons binary mixtures at temperatures from 298.15 K to 318.15 K

rhol	841.64	kg/m3	318.15	Densities, speeds of sound, refractive indices, viscosities and their related thermodynamic properties for n-hexadecane + two aromatic hydrocarbons binary mixtures at temperatures from 298.15 K to 318.15 K	
rhol	849.78	kg/m3	308.15	Densities, speeds of sound, refractive indices, viscosities and their related thermodynamic properties for n-hexadecane + two aromatic hydrocarbons binary mixtures at temperatures from 298.15 K to 318.15 K	
rhol	857.89	kg/m3	298.15	Densities, speeds of sound, refractive indices, viscosities and their related thermodynamic properties for n-hexadecane + two aromatic hydrocarbons binary mixtures at temperatures from 298.15 K to 318.15 K	
rhol	857.95	kg/m3	298.15	Thermodynamic study of 1,1,2,2-tetrachloroethane + hydrocarbon mixtures I. Excess and solvation enthalpies	
rhol	862.00	kg/m3	293.00	KDB	

Correlations

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

Coeff. A	1.36653e+01
Coeff. B	-3.53055e+03
Coeff. C	-6.52710e+01
Temperature range (K), min.	329.18
Temperature range (K), max.	487.90

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.04720e+02
Coeff. B	-9.56288e+03
Coeff. C	-1.31111e+01
Coeff. D	6.52492e-06
Temperature range (K), min.	197.72
Temperature range (K), max.	664.54

Sources

Determination of Henry's Law Constants Using Internal Standards and Solubility Measurements:	https://www.doi.org/10.1021/je3010535
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Saturated Heat Capacities of Some Linear and Branched Alkylbenzenes between (332 and 401) K:	https://www.doi.org/10.1021/je050273f
Measurement and Correlation of Phase Equilibria for Dodecane + sec-Butylbenzene + N-Methyl-2-pyrrolidone:	https://www.doi.org/10.1021/je050191r
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C135988&Units=SI
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=667
Thermodynamic study of 1,1,2,2-tetrachloroethane + hydrocarbon mixtures I. Excess and solvation enthalpies:	https://www.doi.org/10.1016/j.fluid.2006.10.013
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Densities, speeds of sound, refractive indices, viscosities and their related thermodynamic properties for n-hexadecane + two aromatic hydrocarbons binary mixtures at temperatures from 298.15 K to 318.15 K:	https://www.doi.org/10.1016/j.jct.2018.08.036
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Phase equilibria for the extraction of sec-butylbenzene from dodecane with aqueous solutions of N,N-dimethylformamide:	https://www.doi.org/10.1016/j.fluid.2005.12.006
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Liquid Liquid Equilibria of Alkane (C10 C14) + sec-Butylbenzene + Sulfolane:	https://www.doi.org/10.1021/je200203k
Diffusion Coefficients of Isobutylbenzene, sec-Butylbenzene, and 3-Methylbutylbenzene in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je400336p
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=667

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume