Benzene, (2-methylpropyl)-

Other names:	(2-METHYLPROPYL)BENZENE
	1-PHENYL-2-METHYLPROPANE
	1-PHENYLISOBUTANE
	2-Methyl-1-phenylpropane
	2-methylpropylbenzene
	Benzene, isobutyl-
	Isobutylbenzene
	benzene, 2-methylpropyl-
	i-Butylbenzene
Inchi:	InChI=1S/C10H14/c1-9(2)8-10-6-4-3-5-7-10/h3-7,9H,8H2,1-2H3
InchiKey:	KXUHSQYYJYAXGZ-UHFFFAOYSA-N
Formula:	C10H14
SMILES:	CC(C)Cc1ccccc1
Mol. weight [g/mol]:	134.22
CAS:	538-93-2

Physical Properties

Property code	Value	Unit	Source
af	0.3800		KDB
chl	-5866.10 ± 1.00	kJ/mol	NIST Webbook
dm	0.30	debye	KDB
gf	143.29	kJ/mol	Joback Method
hcg	5877.27	kJ/mol	KDB
hcn	5569.741	kJ/mol	KDB
hf	-21.50 ± 1.40	kJ/mol	NIST Webbook
hf	-21.56	kJ/mol	KDB
hfl	-69.90 ± 1.30	kJ/mol	NIST Webbook
hfus	12.17	kJ/mol	Joback Method
hvap	49.50	kJ/mol	NIST Webbook
hvap	48.00	kJ/mol	NIST Webbook
hvap	47.87	kJ/mol	NIST Webbook
hvap	48.40	kJ/mol	NIST Webbook
ie	8.69 ± 0.01	eV	NIST Webbook
ie	8.68	eV	NIST Webbook
ie	8.71 ± 0.05	eV	NIST Webbook
log10ws	-4.12		Estimated Solubility Method

log10ws	-4.12		Aqueous Solubility Prediction Method
logp	2.885		Crippen Method
mcvol	128.000	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=2)		KDB
pc	3050.00 ± 5.88	kPa	NIST Webbook
pc	3050.00	kPa	NIST Webbook
pc	3050.00	kPa	KDB
rinpol	990.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	989.90		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	990.50		NIST Webbook
rinpol	990.90		NIST Webbook
rinpol	994.30		NIST Webbook
rinpol	985.50		NIST Webbook
rinpol	988.30		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	985.20		NIST Webbook
rinpol	985.50		NIST Webbook
rinpol	988.30		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	986.70		NIST Webbook
rinpol	986.70		NIST Webbook
rinpol	982.35		NIST Webbook
rinpol	993.10		NIST Webbook
rinpol	993.10		NIST Webbook
rinpol	989.80		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	1012.00		NIST Webbook
rinpol	1008.20		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	1008.00		NIST Webbook

rinpol	995.70	NIST Webbook
rinpol	996.00	NIST Webbook
rinpol	997.00	NIST Webbook
rinpol	1001.00	NIST Webbook
rinpol	989.50	NIST Webbook
rinpol	1014.90	NIST Webbook
rinpol	1009.00	NIST Webbook
rinpol	997.20	NIST Webbook
rinpol	998.00	NIST Webbook
rinpol	991.30	NIST Webbook
rinpol	992.70	NIST Webbook
rinpol	994.39	NIST Webbook
rinpol	994.48	NIST Webbook
rinpol	994.00	NIST Webbook
rinpol	988.86	NIST Webbook
rinpol	992.41	NIST Webbook
rinpol	994.66	NIST Webbook
rinpol	1004.03	NIST Webbook
rinpol	1007.86	NIST Webbook
rinpol	1010.66	NIST Webbook
rinpol	992.00	NIST Webbook
rinpol	1006.00	NIST Webbook
rinpol	1006.00	NIST Webbook
rinpol	1012.00	NIST Webbook
rinpol	1012.00	NIST Webbook
rinpol	982.00	NIST Webbook
rinpol	993.00	NIST Webbook
rinpol	998.00	NIST Webbook
rinpol	996.00	NIST Webbook
rinpol	1003.00	NIST Webbook
rinpol	998.00	NIST Webbook
rinpol	1012.10	NIST Webbook
rinpol	992.00	NIST Webbook
rinpol	997.00	NIST Webbook
rinpol	1009.00	NIST Webbook
rinpol	994.00	NIST Webbook
rinpol	992.00	NIST Webbook
rinpol	997.00	NIST Webbook
rinpol	992.00	NIST Webbook
ripol	1276.00	NIST Webbook
ripol	1217.00	NIST Webbook
ripol	1270.60	NIST Webbook
ripol	1228.00	NIST Webbook
ripol	1220.00	NIST Webbook

ripol	1241.30		NIST Webbook
ripol	1216.00		NIST Webbook
ripol	1235.90		NIST Webbook
ripol	1215.90		NIST Webbook
ripol	1241.00		NIST Webbook
ripol	1268.00		NIST Webbook
ripol	1204.00		NIST Webbook
ripol	1216.00		NIST Webbook
ripol	1270.60		NIST Webbook
ripol	1250.00		NIST Webbook
ripol	1251.00		NIST Webbook
ripol	1259.00		NIST Webbook
tb	445.94	K	KDB
tc	650.00	K	NIST Webbook
tc	650.00	K	KDB
tc	650.30 ± 3.00	K	NIST Webbook
tc	657.87 ± 0.30	K	NIST Webbook
tf	221.70	K	KDB
vc	0.480	m3/kmol	KDB
zc	0.2708890		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.60	J/mol×K	594.06	Joback Method
cpg	337.41	J/mol×K	663.87	Joback Method
cpg	325.87	J/mol×K	628.97	Joback Method
cpg	256.43	J/mol×K	454.44	Joback Method
cpg	272.00	J/mol×K	489.35	Joback Method
cpg	286.70	J/mol×K	524.25	Joback Method
cpg	300.56	J/mol×K	559.16	Joback Method
dvisc	0.0009050	Pa×s	303.15	Density and Viscosity of Propyl Formate + Aromatic Hydrocarbons at T = (303.15, 308.15, and 313.15) K

dvisc	0.0007840	Pa×s	313.15	Density and Viscosity of Propyl Formate + Aromatic Hydrocarbons at T = (303.15, 308.15, and 313.15) K
dvisc	0.0008480	Pa×s	308.15	Density and Viscosity of Propyl Formate + Aromatic Hydrocarbons at T = (303.15, 308.15, and 313.15) K
dvisc	0.0009050	Pa×s	303.15	Physical Properties of Binary Mixtures of Ethyl Formate with Benzene, Isopropyl Benzene, Isobutyl Benzene, and Butylbenzene at (303.15, 308.15, and 313.15) K
dvisc	0.0008480	Pa×s	308.15	Physical Properties of Binary Mixtures of Ethyl Formate with Benzene, Isopropyl Benzene, Isobutyl Benzene, and Butylbenzene at (303.15, 308.15, and 313.15) K
dvisc	0.0007840	Pa×s	313.15	Physical Properties of Binary Mixtures of Ethyl Formate with Benzene, Isopropyl Benzene, Isobutyl Benzene, and Butylbenzene at (303.15, 308.15, and 313.15) K
hvapt	43.80	kJ/mol	403.50	NIST Webbook
hvapt	43.20	kJ/mol	410.00	NIST Webbook
rfi	1.48397		298.15	Effect of Temperature on the Change of Refractive Index on Mixing for Butyl Acetate + Aromatic Hydrocarbons
rfi	1.48400		298.15	KDB

rhol	853.00	kg/m3	293.00	KDB

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	443.20	K	98.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46312e+01
Coeff. B	-3.97468e+03
Coeff. C	-4.89840e+01
Temperature range (K), min.	326.09
Temperature range (K), max.	475.46

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.00897e+01
Coeff. B	-8.71651e+03
Coeff. C	-1.10159e+01
Coeff. D	6.33426e-06
Temperature range (K), min.	221.70
Temperature range (K), max.	650.15

Datasets

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C538932&Units=SI
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=666
KDB:	https://www.cheric.org/files/research/kdb/mol/mol666.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Prediction and Experimental Measurement of Refractive Index in Ternary Hydrocarbon Mixtures:	https://www.doi.org/10.1021/acs.jced.5b00251
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
Diffusion Coefficients of Isobutylbenzene, sec-Butylbenzene, and 3-Methylbutylbenzene in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je400336p
Comparison between Experimental and Theoretical Estimations of the Thermal Expansion, Concentration Expansion Coefficients, and Viscosity for Binary Mixtures of Ethyl Formate with Benzene, Isopropyl Benzene, Isobutyl Benzene, and Butylbenzene at (303.15, 308.15, and 313.15) K:	https://www.doi.org/10.1021/je8008073
Saturated Heat Capacities of Some Linear and Branched Alkylbenzenes:	https://www.doi.org/10.1021/je050273f
Physical Properties of Binary Mixtures of Ethyl Formate with Benzene, Isopropyl Benzene, Isobutyl Benzene, and Butylbenzene at (303.15, 308.15, and 313.15) K:	https://www.doi.org/10.1021/je900689m
Density and Viscosity of Propyl Formate + Aromatic Hydrocarbons at T = (303.15, 308.15, and 313.15) K:	https://www.doi.org/10.1021/je901071x
Mass Diffusion Coefficient and Soret Coefficient of o-Dichlorobenzene Solutions of PCBM and [60]Fullerene by the Soret Forced Rayleigh Scattering Method:	https://www.doi.org/10.1021/acs.jced.5b00609
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility