Benzene, 1,2,3-trimethyl-

Other names:	1,2,3-TrimethylIbenzene
	1,2,3-Trimethylbenzene
	1,2,3-trimethylbenzene (hemimellitene)
	HEMIMELLITENE
	Hemellitol
Inchi:	InChI=1S/C9H12/c1-7-5-4-6-8(2)9(7)3/h4-6H,1-3H3
InchiKey:	FYGHSUNMUKGBRK-UHFFFAOYSA-N
Formula:	C9H12
SMILES:	Cc1cccc(C)c1C
Mol. weight [g/mol]:	120.19
CAS:	526-73-8

Physical Properties

Property code	Value	Unit	Source
af	0.3660		KDB
chl	-5198.00 ± 1.20	kJ/mol	NIST Webbook
gf	124.60	kJ/mol	KDB
hcg	5198.03	kJ/mol	KDB
hcn	4933.940	kJ/mol	KDB
hf	-9.59	kJ/mol	KDB
hf	-9.60 ± 1.30	kJ/mol	NIST Webbook
hfl	-58.60 ± 1.30	kJ/mol	NIST Webbook
hfus	12.33	kJ/mol	Joback Method
hvap	39.23	kJ/mol	Joback Method
ie	8.42	eV	NIST Webbook
ie	8.60 ± 0.03	eV	NIST Webbook
ie	8.42 ± 0.02	eV	NIST Webbook
ie	8.42 ± 0.02	eV	NIST Webbook
ie	8.48 ± 0.01	eV	NIST Webbook
log10ws	-3.20		Estimated Solubility Method
log10ws	-3.20		Aqueous Solubility Prediction Method
logp	2.612		Crippen Method
mcvol	113.910	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
pc	3454.00	kPa	KDB

pc	3450.00 ± 40.00	kPa	NIST Webbook
pc	3442.60 ± 50.00	kPa	NIST Webbook
pc	3454.00 ± 6.00	kPa	NIST Webbook
rinpol	1011.00		NIST Webbook
rinpol	1002.62		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1019.90		NIST Webbook
rinpol	1008.20		NIST Webbook
rinpol	1016.00		NIST Webbook
rinpol	1005.70		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	162.60		NIST Webbook
rinpol	1011.00		NIST Webbook
rinpol	1009.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1012.40		NIST Webbook
rinpol	1021.90		NIST Webbook
rinpol	1020.50		NIST Webbook
rinpol	1022.90		NIST Webbook
rinpol	1014.60		NIST Webbook
rinpol	1016.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	1035.40		NIST Webbook
rinpol	1043.50		NIST Webbook
rinpol	1001.05		NIST Webbook
rinpol	1015.80		NIST Webbook
rinpol	1022.40		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	1001.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1014.90		NIST Webbook
rinpol	1021.90		NIST Webbook
rinpol	1016.00		NIST Webbook
rinpol	1016.00		NIST Webbook
rinpol	1016.00		NIST Webbook
rinpol	1016.00		NIST Webbook
rinpol	1012.00		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	1016.00		NIST Webbook

rinpol	1013.00	NIST Webbook
rinpol	1017.00	NIST Webbook
rinpol	1010.00	NIST Webbook
rinpol	1012.00	NIST Webbook
rinpol	1009.00	NIST Webbook
rinpol	999.90	NIST Webbook
rinpol	1000.00	NIST Webbook
rinpol	1003.00	NIST Webbook
rinpol	1029.00	NIST Webbook
rinpol	1009.00	NIST Webbook
rinpol	1016.00	NIST Webbook
rinpol	1023.00	NIST Webbook
rinpol	1031.00	NIST Webbook
rinpol	1007.80	NIST Webbook
rinpol	1010.50	NIST Webbook
rinpol	1015.90	NIST Webbook
rinpol	1022.80	NIST Webbook
rinpol	1031.20	NIST Webbook
rinpol	1017.00	NIST Webbook
rinpol	1007.80	NIST Webbook
rinpol	1007.90	NIST Webbook
rinpol	1007.80	NIST Webbook
rinpol	1010.50	NIST Webbook
rinpol	1013.00	NIST Webbook
rinpol	1004.31	NIST Webbook
rinpol	1033.00	NIST Webbook
rinpol	1010.00	NIST Webbook
rinpol	1005.20	NIST Webbook
rinpol	1011.90	NIST Webbook
rinpol	1018.00	NIST Webbook
rinpol	1007.00	NIST Webbook
rinpol	1007.50	NIST Webbook
rinpol	1034.00	NIST Webbook
rinpol	1020.60	NIST Webbook
rinpol	1012.00	NIST Webbook
rinpol	1004.00	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1006.85	NIST Webbook
rinpol	1010.00	NIST Webbook
rinpol	1016.00	NIST Webbook
rinpol	1005.70	NIST Webbook
rinpol	1005.70	NIST Webbook
rinpol	999.00	NIST Webbook
rinpol	1012.00	NIST Webbook

rinpol	1012.40	NIST Webbook
rinpol	1016.00	NIST Webbook
rinpol	1019.90	NIST Webbook
rinpol	1022.70	NIST Webbook
rinpol	1032.80	NIST Webbook
rinpol	1018.00	NIST Webbook
rinpol	1008.20	NIST Webbook
rinpol	1007.00	NIST Webbook
rinpol	1027.00	NIST Webbook
rinpol	979.70	NIST Webbook
rinpol	1016.00	NIST Webbook
rinpol	1019.90	NIST Webbook
rinpol	1022.70	NIST Webbook
rinpol	996.00	NIST Webbook
rinpol	1004.87	NIST Webbook
rinpol	1005.04	NIST Webbook
rinpol	1005.00	NIST Webbook
rinpol	1017.00	NIST Webbook
rinpol	1004.77	NIST Webbook
rinpol	1008.90	NIST Webbook
rinpol	997.82	NIST Webbook
rinpol	1002.62	NIST Webbook
rinpol	1005.67	NIST Webbook
rinpol	1017.96	NIST Webbook
rinpol	1023.11	NIST Webbook
rinpol	1026.55	NIST Webbook
rinpol	1004.00	NIST Webbook
rinpol	1027.65	NIST Webbook
rinpol	1009.00	NIST Webbook
rinpol	1010.00	NIST Webbook
rinpol	1011.00	NIST Webbook
rinpol	1016.00	NIST Webbook
rinpol	1016.00	NIST Webbook
rinpol	1023.00	NIST Webbook
rinpol	1023.00	NIST Webbook
rinpol	1010.00	NIST Webbook
rinpol	162.60	NIST Webbook
rinpol	1016.00	NIST Webbook
rinpol	1007.00	NIST Webbook
rinpol	1016.00	NIST Webbook
rinpol	1015.00	NIST Webbook
rinpol	1017.00	NIST Webbook
rinpol	1009.00	NIST Webbook
rinpol	1020.00	NIST Webbook

rinpol	1023.00	NIST Webbook
rinpol	1014.00	NIST Webbook
rinpol	993.00	NIST Webbook
rinpol	976.00	NIST Webbook
rinpol	997.50	NIST Webbook
rinpol	1034.00	NIST Webbook
rinpol	962.00	NIST Webbook
rinpol	998.00	NIST Webbook
rinpol	1019.00	NIST Webbook
rinpol	1005.00	NIST Webbook
rinpol	1000.00	NIST Webbook
rinpol	1028.20	NIST Webbook
rinpol	966.00	NIST Webbook
rinpol	1016.00	NIST Webbook
rinpol	1000.00	NIST Webbook
rinpol	981.00	NIST Webbook
rinpol	1010.00	NIST Webbook
rinpol	1007.00	NIST Webbook
rinpol	976.00	NIST Webbook
rinpol	1020.00	NIST Webbook
rinpol	1027.00	NIST Webbook
rinpol	1033.00	NIST Webbook
rinpol	981.00	NIST Webbook
rinpol	1022.00	NIST Webbook
rinpol	1006.00	NIST Webbook
rinpol	996.00	NIST Webbook
rinpol	1019.00	NIST Webbook
rinpol	1006.00	NIST Webbook
rinpol	1002.00	NIST Webbook
rinpol	1016.00	NIST Webbook
rinpol	1000.00	NIST Webbook
rinpol	1007.00	NIST Webbook
rinpol	1006.00	NIST Webbook
rinpol	1011.00	NIST Webbook
rinpol	1020.00	NIST Webbook
ripol	1355.00	NIST Webbook
ripol	1340.00	NIST Webbook
ripol	1342.00	NIST Webbook
ripol	1342.00	NIST Webbook
ripol	1343.00	NIST Webbook
ripol	1343.00	NIST Webbook
ripol	1339.00	NIST Webbook
ripol	1337.00	NIST Webbook
ripol	1331.00	NIST Webbook

ripol	1302.00		NIST Webbook
ripol	1341.00		NIST Webbook
ripol	1324.00		NIST Webbook
ripol	1349.00		NIST Webbook
ripol	1332.00		NIST Webbook
ripol	1340.00		NIST Webbook
ripol	1340.00		NIST Webbook
ripol	1369.60		NIST Webbook
ripol	1348.00		NIST Webbook
ripol	1301.80		NIST Webbook
ripol	1320.60		NIST Webbook
ripol	1325.40		NIST Webbook
ripol	1295.00		NIST Webbook
ripol	1382.90		NIST Webbook
ripol	1366.30		NIST Webbook
ripol	1327.00		NIST Webbook
ripol	1355.00		NIST Webbook
ripol	1302.00		NIST Webbook
ripol	1342.00		NIST Webbook
ripol	1337.00		NIST Webbook
ripol	1308.00		NIST Webbook
ripol	1324.00		NIST Webbook
ripol	1344.00		NIST Webbook
ripol	1322.00		NIST Webbook
ripol	1349.00		NIST Webbook
ripol	1348.00		NIST Webbook
ripol	1308.00		NIST Webbook
ripol	1325.00		NIST Webbook
ripol	1355.00		NIST Webbook
ripol	1355.00		NIST Webbook
ripol	1329.00		NIST Webbook
ripol	1325.00		NIST Webbook
ripol	1302.00		NIST Webbook
ripol	1355.00		NIST Webbook
ripol	1355.00		NIST Webbook
ripol	1325.00		NIST Webbook
ripol	1340.00		NIST Webbook
sg	384.84 ± 0.63	J/mol×K	NIST Webbook
sl	267.94	J/mol×K	NIST Webbook
tb	450.00 ± 2.00	K	NIST Webbook
tb	449.27	K	KDB
tb	449.00 ± 3.00	K	NIST Webbook
tb	449.30 ± 0.50	K	NIST Webbook
tb	449.25 ± 0.20	K	NIST Webbook

tb	449.30 ± 0.30	K	NIST Webbook
tb	449.00 ± 6.00	K	NIST Webbook
tb	449.23 ± 0.03	K	NIST Webbook
tb	449.23 ± 0.15	K	NIST Webbook
tb	449.24 ± 0.30	K	NIST Webbook
tb	449.25 ± 0.25	K	NIST Webbook
tb	449.25 ± 0.30	K	NIST Webbook
tb	449.22 ± 0.30	K	NIST Webbook
tb	449.25 ± 0.30	K	NIST Webbook
tb	449.25 ± 0.30	K	NIST Webbook
tb	449.23 ± 0.15	K	NIST Webbook
tb	449.22 ± 0.30	K	NIST Webbook
tb	449.22 ± 0.20	K	NIST Webbook
tb	449.30	K	NIST Webbook
tb	449.25 ± 0.20	K	NIST Webbook
tb	449.25 ± 0.30	K	NIST Webbook
tb	449.55 ± 1.00	K	NIST Webbook
tb	448.40 ± 0.30	K	NIST Webbook
tb	449.24 ± 0.20	K	NIST Webbook
tb	448.00 ± 2.00	K	NIST Webbook
tb	449.25 ± 0.30	K	NIST Webbook
tb	448.25 ± 2.00	K	NIST Webbook
tb	449.00 ± 2.00	K	NIST Webbook
tb	449.24 ± 0.30	K	NIST Webbook
tb	449.23 ± 0.20	K	NIST Webbook
tb	449.25 ± 0.20	K	NIST Webbook
tc	664.50	K	KDB
tc	664.50 ± 0.50	K	NIST Webbook
tc	665.50 ± 1.50	K	NIST Webbook
tc	664.39 ± 0.10	K	NIST Webbook
tc	664.50 ± 0.30	K	NIST Webbook
tf	247.62 ± 0.30	K	NIST Webbook
tf	247.76 ± 0.02	K	NIST Webbook
tf	247.76 ± 0.03	K	NIST Webbook
tf	247.75 ± 0.20	K	NIST Webbook
tf	247.40 ± 0.40	K	NIST Webbook
tf	247.62 ± 0.20	K	NIST Webbook
tf	247.39 ± 0.50	K	NIST Webbook
tf	247.77 ± 0.01	K	NIST Webbook
tf	247.65 ± 0.30	K	NIST Webbook
tf	247.42 ± 1.00	K	NIST Webbook
tf	248.05	K	Aqueous Solubility Prediction Method
tf	247.70	K	KDB
tf	247.62 ± 0.20	K	NIST Webbook

tf	247.74 ± 0.20	K	NIST Webbook
tf	247.75 ± 1.50	K	NIST Webbook
tf	247.65 ± 0.20	K	NIST Webbook
tt	247.81 ± 0.05	K	NIST Webbook
tt	247.80 ± 0.05	K	NIST Webbook
vc	0.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.27	J/mol×K	511.96	Joback Method
cpg	275.86	J/mol×K	616.95	Joback Method
cpg	265.25	J/mol×K	581.96	Joback Method
cpg	254.06	J/mol×K	546.96	Joback Method
cpg	216.81	J/mol×K	441.96	Joback Method
cpg	229.86	J/mol×K	476.96	Joback Method
cpg	285.90	J/mol×K	651.95	Joback Method
cpl	216.44	J/mol×K	298.15	NIST Webbook
dvisc	0.0003221	Pa×s	375.52	Joback Method
dvisc	0.0002545	Pa×s	408.74	Joback Method
dvisc	0.0002083	Pa×s	441.96	Joback Method
dvisc	0.0004268	Pa×s	342.31	Joback Method
dvisc	0.0006008	Pa×s	309.09	Joback Method
dvisc	0.0009182	Pa×s	275.87	Joback Method
dvisc	0.0015760	Pa×s	242.65	Joback Method
hfust	8.18	kJ/mol	247.80	NIST Webbook
hfust	1.33	kJ/mol	230.30	NIST Webbook
hfust	0.66	kJ/mol	218.70	NIST Webbook
hfust	8.18	kJ/mol	247.80	NIST Webbook
hvapt	44.80	kJ/mol	409.50	NIST Webbook
hvapt	40.04	kJ/mol	449.30	KDB
hvapt	42.50	kJ/mol	264.50	NIST Webbook
rfi	1.51150		298.15	KDB
rhol	894.00	kg/m3	293.00	KDB
sfust	33.01	J/mol×K	247.80	NIST Webbook
sfust	3.00	J/mol×K	218.70	NIST Webbook
sfust	5.80	J/mol×K	230.30	NIST Webbook
srf	0.03	N/m	293.20	KDB

tcondl	0.13	W/m×K	313.04	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.13	W/m×K	312.79	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.13	W/m×K	295.99	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.13	W/m×K	313.21	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.12	W/m×K	330.74	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	

tcondl	0.12	W/m×K	330.99	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.12	W/m×K	331.17	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.13	W/m×K	295.81	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.13	W/m×K	295.58	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.13	W/m×K	283.74	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	

tcondl	0.13	W/m×K	283.57	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.13	W/m×K	276.73	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.13	W/m×K	276.58	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.13	W/m×K	276.36	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.13	W/m×K	257.99	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	

tcondl	0.13	W/m×K	257.83	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.13	W/m×K	257.62	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.13	W/m×K	283.35	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47893e+01
Coeff. B	-4.12083e+03
Coeff. C	-4.41160e+01
Temperature range (K), min.	328.28
Temperature range (K), max.	478.90

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2

Coeff. A	6.06633e+01
Coeff. B	-7.50148e+03
Coeff. C	-6.53516e+00
Coeff. D	2.76776e-06
Temperature range (K), min.	247.79
Temperature range (K), max.	664.53

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C526738&Units=SI
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons:	https://www.doi.org/10.1021/je034162x
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=662
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB:	https://www.cheric.org/files/research/kdb/mol/mol662.mol

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
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
nfpaf:	NFPA Fire Rating
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
sg:	Molar entropy at standard conditions
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume