Benzene, 1-methyl-2-propyl-

Other names:	1-Methyl-2-n-propylbenzene
	1-Methyl-2-propylbenzene
	2-Propyltoluene
	2-n-Propyltoluene
	O-METHYLPROPYLBENZENE
	O-PROPYLTOLUENE
	Toluene, o-propyl-
Inchi:	InChI=1S/C10H14/c1-3-6-10-8-5-4-7-9(10)2/h4-5,7-8H,3,6H2,1-2H3
InchiKey:	YQZBFMJOASEONC-UHFFFAOYSA-N
Formula:	C10H14
SMILES:	CCCc1ccccc1C
Mol. weight [g/mol]:	134.22
CAS:	1074-17-5

Physical Properties

Property code	Value	Unit	Source
af	0.3990		KDB
chl	-5862.70 ± 2.20	kJ/mol	NIST Webbook
chl	-5863.46 ± 0.88	kJ/mol	NIST Webbook
gf	136.10	kJ/mol	Joback Method
hf	-24.67	kJ/mol	Joback Method
hfl	-73.30 ± 2.10	kJ/mol	NIST Webbook
hfl	-72.50 ± 1.00	kJ/mol	NIST Webbook
hfus	15.31	kJ/mol	Joback Method
hvap	52.70	kJ/mol	NIST Webbook
log10ws	-3.17		Crippen Method
logp	2.948		Crippen Method
mcvol	128.000	ml/mol	McGowan Method
pc	2964.00	kPa	KDB
rinpol	1049.00		NIST Webbook
rinpol	1057.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1048.00		NIST Webbook
rinpol	1074.10		NIST Webbook
rinpol	1054.00		NIST Webbook
rinpol	1058.00		NIST Webbook

rinpol	1048.00	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1061.00	NIST Webbook
rinpol	1058.00	NIST Webbook
rinpol	1057.00	NIST Webbook
rinpol	1046.10	NIST Webbook
rinpol	1050.00	NIST Webbook
rinpol	172.80	NIST Webbook
rinpol	1058.80	NIST Webbook
rinpol	1067.00	NIST Webbook
rinpol	1053.00	NIST Webbook
rinpol	1057.85	NIST Webbook
rinpol	1065.00	NIST Webbook
rinpol	1058.00	NIST Webbook
rinpol	1063.00	NIST Webbook
rinpol	1056.70	NIST Webbook
rinpol	1044.00	NIST Webbook
rinpol	1045.00	NIST Webbook
rinpol	1059.00	NIST Webbook
rinpol	1059.00	NIST Webbook
rinpol	1057.50	NIST Webbook
rinpol	1057.00	NIST Webbook
rinpol	1057.00	NIST Webbook
rinpol	1057.00	NIST Webbook
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rinpol	1047.00	NIST Webbook
rinpol	1048.30	NIST Webbook
rinpol	1059.00	NIST Webbook
rinpol	1065.00	NIST Webbook
rinpol	1073.00	NIST Webbook
rinpol	1042.00	NIST Webbook
rinpol	1045.40	NIST Webbook
rinpol	1059.00	NIST Webbook
rinpol	1065.40	NIST Webbook
rinpol	1072.90	NIST Webbook
rinpol	1045.80	NIST Webbook
rinpol	1039.40	NIST Webbook
rinpol	1042.00	NIST Webbook
rinpol	1045.40	NIST Webbook
rinpol	1046.00	NIST Webbook
rinpol	1055.00	NIST Webbook
rinpol	1069.00	NIST Webbook
rinpol	1074.00	NIST Webbook

rinpol	1079.00	NIST Webbook
rinpol	1073.00	NIST Webbook
rinpol	1080.00	NIST Webbook
rinpol	1085.00	NIST Webbook
rinpol	1089.00	NIST Webbook
rinpol	1046.00	NIST Webbook
rinpol	1045.80	NIST Webbook
rinpol	1046.30	NIST Webbook
rinpol	1045.00	NIST Webbook
rinpol	1051.00	NIST Webbook
rinpol	1050.50	NIST Webbook
rinpol	1042.00	NIST Webbook
rinpol	1075.20	NIST Webbook
rinpol	1050.00	NIST Webbook
rinpol	1079.00	NIST Webbook
rinpol	1057.85	NIST Webbook
rinpol	1057.00	NIST Webbook
rinpol	1049.00	NIST Webbook
rinpol	1055.00	NIST Webbook
rinpol	1058.80	NIST Webbook
rinpol	1048.90	NIST Webbook
rinpol	1052.50	NIST Webbook
rinpol	1052.22	NIST Webbook
rinpol	1052.67	NIST Webbook
rinpol	1053.00	NIST Webbook
rinpol	1050.00	NIST Webbook
rinpol	1065.00	NIST Webbook
rinpol	1058.00	NIST Webbook
rinpol	1059.00	NIST Webbook
rinpol	1065.00	NIST Webbook
rinpol	1065.00	NIST Webbook
rinpol	1035.00	NIST Webbook
rinpol	1049.00	NIST Webbook
rinpol	1039.41	NIST Webbook
rinpol	1060.00	NIST Webbook
ripol	1342.00	NIST Webbook
ripol	1305.40	NIST Webbook
ripol	1321.50	NIST Webbook
ripol	1305.40	NIST Webbook
ripol	1299.00	NIST Webbook
ripol	1330.00	NIST Webbook
ripol	1342.00	NIST Webbook
ripol	1328.00	NIST Webbook
ripol	1313.00	NIST Webbook

ripol	1305.00		NIST Webbook
ripol	1328.00		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1329.00		NIST Webbook
ripol	1384.00		NIST Webbook
ripol	1368.00		NIST Webbook
ripol	1355.00		NIST Webbook
ripol	1327.70		NIST Webbook
tb	548.20	K	KDB
tc	672.50	K	KDB
tf	212.71 ± 0.20	K	NIST Webbook
tf	212.95	K	KDB
tf	212.84 ± 0.01	K	NIST Webbook
vc	0.490	m3/kmol	KDB
zc	0.2596380		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.27	J/mol×K	631.46	Joback Method
cpg	311.49	J/mol×K	597.14	Joback Method
cpg	299.03	J/mol×K	562.82	Joback Method
cpg	285.87	J/mol×K	528.50	Joback Method
cpg	271.96	J/mol×K	494.18	Joback Method
cpg	257.29	J/mol×K	459.86	Joback Method
cpg	334.39	J/mol×K	665.78	Joback Method
dvisc	0.0024545	Pa×s	241.40	Joback Method
dvisc	0.0002163	Pa×s	459.86	Joback Method
dvisc	0.0002725	Pa×s	423.45	Joback Method
dvisc	0.0003585	Pa×s	387.04	Joback Method
dvisc	0.0004992	Pa×s	350.63	Joback Method
dvisc	0.0007506	Pa×s	314.22	Joback Method
dvisc	0.0012559	Pa×s	277.81	Joback Method
hvapt	48.00	kJ/mol	412.50	NIST Webbook
rhol	872.44	kg/m3	293.10	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44694e+01
Coeff. B	-3.86967e+03
Coeff. C	-6.51320e+01
Temperature range (K), min.	337.99
Temperature range (K), max.	487.68

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.06243e+02
Coeff. B	-9.80205e+03
Coeff. C	-1.33532e+01
Coeff. D	7.58129e-06
Temperature range (K), min.	337.15
Temperature range (K), max.	488.15

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol669.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1074175&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=669

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

Legend

af: Acentric Factor

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
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
zc:	Critical Compressibility