Benzene, 1-methyl-4-propyl-

Other names:	1-Methyl-4-n-propylbenzene
	1-Methyl-4-propylbenzene
	4-Propyl-1-methylbenzene
	4-n-Propyltoluene
	4-propyltoluene
	P-METHYLPROPYLBENZENE
	P-PROPYLTOLUENE
	Toluene, p-propyl-
	p-n-Propyl toluene
Inchi:	InChI=1S/C10H14/c1-3-4-10-7-5-9(2)6-8-10/h5-8H,3-4H2,1-2H3
InchiKey:	JXFVMNFKABWTHD-UHFFFAOYSA-N
Formula:	C10H14
SMILES:	CCCc1ccc(C)cc1
Mol. weight [g/mol]:	134.22
CAS:	1074-55-1

Physical Properties

Property code	Value	Unit	Source
af	0.4020		KDB
chl	-5860.40 ± 2.20	kJ/mol	NIST Webbook
chl	-5860.86 ± 0.88	kJ/mol	NIST Webbook
gf	136.10	kJ/mol	Joback Method
hf	-24.67	kJ/mol	Joback Method
hfl	-75.60 ± 2.10	kJ/mol	NIST Webbook
hfl	-75.10 ± 1.00	kJ/mol	NIST Webbook
hfus	15.31	kJ/mol	Joback Method
hvap	51.90	kJ/mol	NIST Webbook
log10ws	-3.17		Crippen Method
logp	2.948		Crippen Method
mcvol	128.000	ml/mol	McGowan Method
pc	2845.00	kPa	KDB
rinpol	1032.00		NIST Webbook
rinpol	1046.00		NIST Webbook
rinpol	1046.00		NIST Webbook
rinpol	1046.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1047.00		NIST Webbook

rinpol	1047.00	NIST Webbook
rinpol	1040.00	NIST Webbook
rinpol	1038.10	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1053.00	NIST Webbook
rinpol	1058.00	NIST Webbook
rinpol	1035.90	NIST Webbook
rinpol	1038.80	NIST Webbook
rinpol	1047.50	NIST Webbook
rinpol	1052.60	NIST Webbook
rinpol	1057.70	NIST Webbook
rinpol	1035.40	NIST Webbook
rinpol	1033.00	NIST Webbook
rinpol	1035.90	NIST Webbook
rinpol	1038.80	NIST Webbook
rinpol	1040.00	NIST Webbook
rinpol	1033.02	NIST Webbook
rinpol	1035.40	NIST Webbook
rinpol	1039.30	NIST Webbook
rinpol	1039.00	NIST Webbook
rinpol	1044.00	NIST Webbook
rinpol	1039.00	NIST Webbook
rinpol	1070.00	NIST Webbook
rinpol	1046.40	NIST Webbook
rinpol	1046.00	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1038.40	NIST Webbook
rinpol	1040.00	NIST Webbook
rinpol	1042.00	NIST Webbook
rinpol	1036.49	NIST Webbook
rinpol	1039.82	NIST Webbook
rinpol	1042.19	NIST Webbook
rinpol	1052.90	NIST Webbook
rinpol	1056.46	NIST Webbook
rinpol	1059.10	NIST Webbook
rinpol	1039.00	NIST Webbook
rinpol	1046.00	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1053.00	NIST Webbook
rinpol	1053.00	NIST Webbook
rinpol	1046.50	NIST Webbook
rinpol	1047.00	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1046.00	NIST Webbook

rinpol	1056.00	NIST Webbook
rinpol	1059.00	NIST Webbook
rinpol	1049.00	NIST Webbook
rinpol	1061.30	NIST Webbook
rinpol	1047.00	NIST Webbook
rinpol	1038.00	NIST Webbook
rinpol	1046.00	NIST Webbook
rinpol	1038.00	NIST Webbook
rinpol	1038.00	NIST Webbook
rinpol	1046.00	NIST Webbook
rinpol	1038.00	NIST Webbook
rinpol	1047.00	NIST Webbook
rinpol	1046.50	NIST Webbook
rinpol	1047.00	NIST Webbook
rinpol	1032.00	NIST Webbook
rinpol	172.80	NIST Webbook
rinpol	1046.40	NIST Webbook
rinpol	1046.00	NIST Webbook
rinpol	1047.00	NIST Webbook
rinpol	1058.00	NIST Webbook
rinpol	1057.70	NIST Webbook
rinpol	1040.00	NIST Webbook
rinpol	1044.00	NIST Webbook
rinpol	172.80	NIST Webbook
rinpol	1046.00	NIST Webbook
rinpol	1039.80	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1046.00	NIST Webbook
ripol	1295.00	NIST Webbook
ripol	1279.90	NIST Webbook
ripol	1296.00	NIST Webbook
ripol	1279.90	NIST Webbook
ripol	1295.00	NIST Webbook
ripol	1297.00	NIST Webbook
ripol	1314.00	NIST Webbook
ripol	1315.00	NIST Webbook
ripol	1326.00	NIST Webbook
ripol	1338.00	NIST Webbook
ripol	1354.00	NIST Webbook
ripol	1302.00	NIST Webbook
ripol	1280.00	NIST Webbook
ripol	1301.00	NIST Webbook
ripol	1280.00	NIST Webbook
ripol	1287.50	NIST Webbook

ripol	1262.00		NIST Webbook
ripol	1301.00		NIST Webbook
ripol	1262.00		NIST Webbook
tb	456.20	K	KDB
tc	660.70	K	KDB
tf	209.55	K	KDB
tf	208.95 ± 0.50	K	NIST Webbook
tf	209.38 ± 0.20	K	NIST Webbook
tf	209.45 ± 0.01	K	NIST Webbook
tf	208.50 ± 0.60	K	NIST Webbook
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.39	J/mol×K	665.78	Joback Method
cpg	257.29	J/mol×K	459.86	Joback Method
cpg	271.96	J/mol×K	494.18	Joback Method
cpg	285.87	J/mol×K	528.50	Joback Method
cpg	299.03	J/mol×K	562.82	Joback Method
cpg	311.49	J/mol×K	597.14	Joback Method
cpg	323.27	J/mol×K	631.46	Joback Method
dvisc	0.0002163	Pa×s	459.86	Joback Method
dvisc	0.0024545	Pa×s	241.40	Joback Method
dvisc	0.0012559	Pa×s	277.81	Joback Method
dvisc	0.0007506	Pa×s	314.22	Joback Method
dvisc	0.0004992	Pa×s	350.63	Joback Method
dvisc	0.0003585	Pa×s	387.04	Joback Method
dvisc	0.0002725	Pa×s	423.45	Joback Method
hvapt	47.60	kJ/mol	411.00	NIST Webbook
rhol	859.01	kg/m3	293.10	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45089e+01

Coeff. B	-3.90155e+03
Coeff. C	-6.19770e+01
Temperature range (K), min.	336.32
Temperature range (K), max.	486.18

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.04171e+02
Coeff. B	-9.64433e+03
Coeff. C	-1.30610e+01
Coeff. D	7.46048e-06
Temperature range (K), min.	335.15
Temperature range (K), max.	487.15

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1074551&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=671

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol671.mol

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

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