Benzene, 1,2,3,4-tetramethyl-

Other names:	1,2,3,4-Tetramethylbenzene
	PREHNITENE
	PREHNITOL
Inchi:	InChI=1S/C10H14/c1-7-5-6-8(2)10(4)9(7)3/h5-6H,1-4H3
InchiKey:	UOHMMEJUHBCKEE-UHFFFAOYSA-N
Formula:	C10H14
SMILES:	Cc1ccc(C)c(C)c1C
Mol. weight [g/mol]:	134.22
CAS:	488-23-3

Physical Properties

Property code	Value	Unit	Source
chl	-5839.60 ± 3.00	kJ/mol	NIST Webbook
chl	-5827.50 ± 5.90	kJ/mol	NIST Webbook
chl	-5845.70 ± 1.10	kJ/mol	NIST Webbook
gf	116.84	kJ/mol	Joback Method
hf	-43.80 ± 3.00	kJ/mol	NIST Webbook
hf	-36.00 ± 1.40	kJ/mol	NIST Webbook
hf	-37.60 ± 1.20	kJ/mol	NIST Webbook
hfl	-90.20 ± 1.20	kJ/mol	NIST Webbook
hfl	-96.40 ± 3.00	kJ/mol	NIST Webbook
hfus	14.53	kJ/mol	Joback Method
hvap	57.20	kJ/mol	NIST Webbook
hvap	52.60 ± 0.20	kJ/mol	NIST Webbook
hvap	52.56 ± 0.17	kJ/mol	NIST Webbook
hvap	54.00	kJ/mol	NIST Webbook
ie	8.14	eV	NIST Webbook
ie	8.14	eV	NIST Webbook
ie	8.18	eV	NIST Webbook
log10ws	-3.37		Crippen Method
logp	2.920		Crippen Method
mcvol	128.000	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
rinpol	1144.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1136.00		NIST Webbook

rinpol	1125.60	NIST Webbook
rinpol	1150.40	NIST Webbook
rinpol	1133.00	NIST Webbook
rinpol	1187.00	NIST Webbook
rinpol	1147.00	NIST Webbook
rinpol	1142.00	NIST Webbook
rinpol	1120.00	NIST Webbook
rinpol	1122.00	NIST Webbook
rinpol	1145.30	NIST Webbook
rinpol	1149.90	NIST Webbook
rinpol	1148.20	NIST Webbook
rinpol	1144.20	NIST Webbook
rinpol	1149.90	NIST Webbook
rinpol	1153.80	NIST Webbook
rinpol	1175.20	NIST Webbook
rinpol	1144.20	NIST Webbook
rinpol	1149.90	NIST Webbook
rinpol	1153.80	NIST Webbook
rinpol	1149.90	NIST Webbook
rinpol	1148.20	NIST Webbook
rinpol	1135.84	NIST Webbook
rinpol	1136.00	NIST Webbook
rinpol	1133.00	NIST Webbook
rinpol	1160.00	NIST Webbook
rinpol	1142.00	NIST Webbook
rinpol	1127.00	NIST Webbook
rinpol	1142.00	NIST Webbook
rinpol	1142.00	NIST Webbook
rinpol	1148.00	NIST Webbook
rinpol	1147.00	NIST Webbook
rinpol	1162.00	NIST Webbook
rinpol	1151.00	NIST Webbook
rinpol	1153.00	NIST Webbook
rinpol	1149.00	NIST Webbook
rinpol	1144.00	NIST Webbook
rinpol	1161.40	NIST Webbook
rinpol	1125.98	NIST Webbook
rinpol	1132.00	NIST Webbook
rinpol	1145.00	NIST Webbook
rinpol	1151.00	NIST Webbook
rinpol	1128.00	NIST Webbook
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rinpol	1125.98	NIST Webbook
rinpol	1125.60	NIST Webbook
rinpol	1144.00	NIST Webbook
rinpol	1150.40	NIST Webbook
rinpol	1145.00	NIST Webbook
rinpol	1135.00	NIST Webbook
rinpol	1148.00	NIST Webbook
rinpol	1149.00	NIST Webbook
rinpol	1147.00	NIST Webbook
rinpol	1139.00	NIST Webbook
rinpol	1132.70	NIST Webbook
rinpol	1129.20	NIST Webbook
rinpol	1135.00	NIST Webbook
rinpol	1129.20	NIST Webbook
rinpol	1127.50	NIST Webbook
rinpol	1139.00	NIST Webbook
rinpol	1139.00	NIST Webbook
rinpol	1139.00	NIST Webbook
rinpol	1139.00	NIST Webbook
rinpol	1140.90	NIST Webbook
rinpol	1169.40	NIST Webbook
rinpol	1159.80	NIST Webbook
rinpol	1136.00	NIST Webbook
rinpol	1130.00	NIST Webbook
rinpol	1132.70	NIST Webbook
ripol	1462.00	NIST Webbook
ripol	1505.10	NIST Webbook
ripol	1505.10	NIST Webbook
ripol	1461.60	NIST Webbook
ripol	1456.00	NIST Webbook
ripol	1434.70	NIST Webbook
ripol	1436.00	NIST Webbook
ripol	1430.00	NIST Webbook
ripol	1462.00	NIST Webbook
ripol	1495.00	NIST Webbook
ripol	1435.00	NIST Webbook
ripol	1462.00	NIST Webbook
ripol	1464.00	NIST Webbook
ripol	1476.00	NIST Webbook

ripol	1493.00		NIST Webbook
sl	290.80	J/mol×K	NIST Webbook
tb	469.82	K	Joback Method
tc	678.39	K	Joback Method
tf	266.75 ± 0.10	K	NIST Webbook
tf	266.82 ± 0.20	K	NIST Webbook
tf	265.50 ± 1.00	K	NIST Webbook
tf	265.75 ± 2.50	K	NIST Webbook
tt	265.40 ± 0.30	K	NIST Webbook
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.58	J/mol×K	643.63	Joback Method
cpg	258.77	J/mol×K	469.82	Joback Method
cpg	272.57	J/mol×K	504.58	Joback Method
cpg	285.73	J/mol×K	539.34	Joback Method
cpg	298.28	J/mol×K	574.11	Joback Method
cpg	310.23	J/mol×K	608.87	Joback Method
cpg	332.37	J/mol×K	678.39	Joback Method
cpl	236.00	J/mol×K	291.90	NIST Webbook
cpl	244.30	J/mol×K	298.00	NIST Webbook
dvisc	0.0001983	Pa×s	469.82	Joback Method
dvisc	0.0012469	Pa×s	266.44	Joback Method
dvisc	0.0007720	Pa×s	300.34	Joback Method
dvisc	0.0005268	Pa×s	334.23	Joback Method
dvisc	0.0003857	Pa×s	368.13	Joback Method
dvisc	0.0002977	Pa×s	402.03	Joback Method
dvisc	0.0002391	Pa×s	435.92	Joback Method
hfust	11.23	kJ/mol	265.40	NIST Webbook
hfust	11.23	kJ/mol	265.40	NIST Webbook
hfust	11.23	kJ/mol	265.40	NIST Webbook
hvapt	55.70	kJ/mol	396.50	NIST Webbook
hvapt	50.70	kJ/mol	430.50	NIST Webbook
sfust	42.30	J/mol×K	265.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46818e+01
Coeff. B	-4.16744e+03
Coeff. C	-6.40760e+01
Temperature range (K), min.	353.60
Temperature range (K), max.	508.82

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.69035e+01
Coeff. B	-9.94657e+03
Coeff. C	-1.17674e+01
Coeff. D	4.88689e-06
Temperature range (K), min.	352.15
Temperature range (K), max.	695.10

Sources

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/mol684.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C488233&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=684

Legend

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
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
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume