Benzene, 1,2,4,5-tetramethyl-

Other names:	1,2,4,5-Tetramethylbenzene
	DURENE
	DUROL
	p-Xylene, 2,5-dimethyl-
Inchi:	InChI=1S/C10H14/c1-7-5-9(3)10(4)6-8(7)2/h5-6H,1-4H3
InchiKey:	SQNZJJAZBFDUTD-UHFFFAOYSA-N
Formula:	C10H14
SMILES:	Cc1cc(C)c(C)cc1C
Mol. weight [g/mol]:	134.22
CAS:	95-93-2

Physical Properties

Property code	Value	Unit	Source
af	0.4350		KDB
chl	-5837.30 ± 3.00	kJ/mol	NIST Webbook
chl	-5809.10 ± 5.90	kJ/mol	NIST Webbook
chs	-5816.10 ± 1.20	kJ/mol	NIST Webbook
chs	-5814.20 ± 1.40	kJ/mol	NIST Webbook
ea	0.05 ± 0.02	eV	NIST Webbook
gf	119.50	kJ/mol	KDB
hf	-47.10 ± 1.90	kJ/mol	NIST Webbook
hf	-46.90 ± 1.80	kJ/mol	NIST Webbook
hf	-45.30	kJ/mol	NIST Webbook
hf	-45.30	kJ/mol	KDB
hfl	-98.70 ± 3.00	kJ/mol	NIST Webbook
hfs	-121.70 ± 1.90	kJ/mol	NIST Webbook
hfs	-119.90 ± 1.30	kJ/mol	NIST Webbook
hfus	14.53	kJ/mol	Joback Method
hvap	42.12	kJ/mol	Joback Method
ie	8.03	eV	NIST Webbook
ie	8.05	eV	NIST Webbook
ie	8.37	eV	NIST Webbook
ie	8.06 ± 0.03	eV	NIST Webbook
ie	8.07	eV	NIST Webbook
ie	8.50 ± 0.05	eV	NIST Webbook
ie	8.05	eV	NIST Webbook
ie	8.03 ± 0.01	eV	NIST Webbook

ie	8.13	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
ie	8.05 ± 0.02	eV	NIST Webbook
log10ws	-4.59		Aqueous Solubility Prediction Method
log10ws	-4.59		Estimated Solubility Method
logp	2.920		Crippen Method
mcvol	128.000	ml/mol	McGowan Method
pc	2900.00	kPa	KDB
pc	2897.90 ± 151.99	kPa	NIST Webbook
pc	2900.00	kPa	NIST Webbook
rinpol	1124.70		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1132.40		NIST Webbook
rinpol	1109.30		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1116.70		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1106.10		NIST Webbook
rinpol	1105.60		NIST Webbook
rinpol	1106.50		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1113.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1105.00		NIST Webbook

rinpol	1108.00	NIST Webbook
rinpol	1100.00	NIST Webbook
rinpol	1096.40	NIST Webbook
rinpol	1118.00	NIST Webbook
rinpol	1100.00	NIST Webbook
rinpol	1107.00	NIST Webbook
rinpol	1114.00	NIST Webbook
rinpol	1121.00	NIST Webbook
rinpol	1102.80	NIST Webbook
rinpol	1105.90	NIST Webbook
rinpol	1107.20	NIST Webbook
rinpol	1114.40	NIST Webbook
rinpol	1121.20	NIST Webbook
rinpol	1106.00	NIST Webbook
rinpol	1102.80	NIST Webbook
rinpol	1105.90	NIST Webbook
rinpol	1107.00	NIST Webbook
rinpol	1099.53	NIST Webbook
rinpol	1131.00	NIST Webbook
rinpol	1128.00	NIST Webbook
rinpol	1134.00	NIST Webbook
rinpol	1094.90	NIST Webbook
rinpol	1145.00	NIST Webbook
rinpol	1123.00	NIST Webbook
rinpol	1114.20	NIST Webbook
rinpol	1147.00	NIST Webbook
rinpol	1104.85	NIST Webbook
rinpol	1108.00	NIST Webbook
rinpol	1129.00	NIST Webbook
rinpol	1109.00	NIST Webbook
rinpol	1117.00	NIST Webbook
rinpol	1109.40	NIST Webbook
rinpol	1109.70	NIST Webbook
rinpol	1114.10	NIST Webbook
rinpol	1115.80	NIST Webbook
rinpol	1130.20	NIST Webbook
rinpol	1140.00	NIST Webbook
rinpol	1097.90	NIST Webbook
rinpol	1101.20	NIST Webbook
rinpol	1109.70	NIST Webbook
rinpol	1114.10	NIST Webbook
rinpol	1115.80	NIST Webbook
rinpol	1101.84	NIST Webbook
rinpol	1102.07	NIST Webbook

rinpol	1102.00	NIST Webbook
rinpol	1099.00	NIST Webbook
rinpol	1099.00	NIST Webbook
rinpol	1110.08	NIST Webbook
rinpol	1107.00	NIST Webbook
rinpol	1121.00	NIST Webbook
rinpol	1107.00	NIST Webbook
rinpol	1107.00	NIST Webbook
rinpol	1114.00	NIST Webbook
rinpol	1114.00	NIST Webbook
rinpol	1111.00	NIST Webbook
rinpol	1103.00	NIST Webbook
rinpol	1111.00	NIST Webbook
rinpol	1117.00	NIST Webbook
rinpol	1113.00	NIST Webbook
rinpol	1111.00	NIST Webbook
rinpol	1109.00	NIST Webbook
rinpol	1116.00	NIST Webbook
rinpol	1118.00	NIST Webbook
rinpol	1112.00	NIST Webbook
rinpol	1101.00	NIST Webbook
rinpol	1100.00	NIST Webbook
rinpol	1123.20	NIST Webbook
rinpol	1113.00	NIST Webbook
rinpol	1098.00	NIST Webbook
rinpol	1102.00	NIST Webbook
rinpol	1130.00	NIST Webbook
rinpol	1119.00	NIST Webbook
rinpol	1124.00	NIST Webbook
rinpol	1096.00	NIST Webbook
rinpol	1103.00	NIST Webbook
ripol	1406.80	NIST Webbook
ripol	1447.30	NIST Webbook
ripol	1463.00	NIST Webbook
ripol	1480.30	NIST Webbook
ripol	1446.00	NIST Webbook
ripol	1459.00	NIST Webbook
ripol	1435.00	NIST Webbook
ripol	1435.00	NIST Webbook
ripol	1407.00	NIST Webbook
ripol	1411.00	NIST Webbook
ripol	1400.00	NIST Webbook
ripol	1440.00	NIST Webbook
ripol	1433.00	NIST Webbook

ripol	1432.00		NIST Webbook
ripol	1438.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1419.00		NIST Webbook
ripol	1445.80		NIST Webbook
ripol	1401.30		NIST Webbook
ripol	1416.00		NIST Webbook
sl	245.60	J/mol×K	NIST Webbook
tb	469.99	K	KDB
tc	675.65 ± 2.00	K	NIST Webbook
tc	676.00	K	NIST Webbook
tc	676.00	K	KDB
tf	352.40	K	KDB
tf	352.58	K	Aqueous Solubility Prediction Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.23	J/mol×K	608.87	Joback Method
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	332.37	J/mol×K	678.39	Joback Method
cpl	215.10	J/mol×K	297.10	NIST Webbook
cpl	275.70	J/mol×K	353.00	NIST Webbook
cpl	220.10	J/mol×K	298.10	NIST Webbook
cps	215.60	J/mol×K	303.15	NIST Webbook
cps	204.02	J/mol×K	298.15	NIST Webbook
dvisc	0.0012469	Pa×s	266.44	Joback Method
dvisc	0.0002977	Pa×s	402.03	Joback Method
dvisc	0.0003857	Pa×s	368.13	Joback Method
dvisc	0.0005268	Pa×s	334.23	Joback Method
dvisc	0.0007720	Pa×s	300.34	Joback Method
dvisc	0.0001983	Pa×s	469.82	Joback Method
dvisc	0.0002391	Pa×s	435.92	Joback Method
hfust	21.34	kJ/mol	352.05	NIST Webbook
hfust	20.88	kJ/mol	352.40	NIST Webbook

hfust	20.88	kJ/mol	352.40	NIST Webbook
hfust	20.88	kJ/mol	352.40	NIST Webbook
hsubt	71.30	kJ/mol	333.00	NIST Webbook
hvapt	45.52	kJ/mol	470.00	KDB
hvapt	47.70 ± 0.30	kJ/mol	372.00	NIST Webbook
hvapt	49.40	kJ/mol	426.50	NIST Webbook
rfi	1.50930		298.15	KDB
rhol	838.00	kg/m3	354.00	KDB
sfust	59.30	J/mol×K	352.40	NIST Webbook
srf	0.02	N/m	373.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47415e+01
Coeff. B	-4.16711e+03
Coeff. C	-5.83480e+01
Temperature range (K), min.	346.65
Temperature range (K), max.	500.25

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.09017e+02
Coeff. B	-1.02916e+04
Coeff. C	-1.36620e+01
Coeff. D	7.04044e-06
Temperature range (K), min.	352.38
Temperature range (K), max.	675.15

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=686

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95932&Units=SI
Vapor-Liquid Equilibrium of Durene in Methanol or Ethanol:	https://www.doi.org/10.1021/je034227w
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/files/research/kdb/mol/mol686.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation 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
rfi:	Refractive Index
rhol:	Liquid Density
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
srf:	Surface Tension
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume