Benzene, 1,2,3,5-tetramethyl-

Other names: 1,2,3,5-Tetramethylbenzene
ISODURENE
Inchi: InChI=1S/C10H14/c1-7-5-8(2)10(4)9(3)6-7/h5-6H,1-4H3
InchiKey: BFIMMTCNYPIMRN-UHFFFAOYSA-N
Formula: C10H14
SMILES: Cc1cc(C)c(C)c(C)c1
Mol. weight [g/mol]: 134.22
CAS: 527-53-7

Physical Properties

Property code	Value	Unit	Source
af	0.4120		KDB
affp	845.60	kJ/mol	NIST Webbook
basg	816.50	kJ/mol	NIST Webbook
chl	-5837.50 ± 3.00	kJ/mol	NIST Webbook
chl	-5839.60 ± 1.10	kJ/mol	NIST Webbook
chl	-5815.30 ± 5.90	kJ/mol	NIST Webbook
ea	0.11 ± 0.01	eV	NIST Webbook
gf	118.80	kJ/mol	KDB
hf	-44.40 ± 1.20	kJ/mol	NIST Webbook
hf	-46.50 ± 3.00	kJ/mol	NIST Webbook
hf	-43.20 ± 1.30	kJ/mol	NIST Webbook
hf	-44.84	kJ/mol	KDB
hfl	-96.40 ± 1.20	kJ/mol	NIST Webbook
hfl	-98.50 ± 3.00	kJ/mol	NIST Webbook
hfus	14.53	kJ/mol	Joback Method
hvap	51.98 ± 0.17	kJ/mol	NIST Webbook
hvap	52.00 ± 0.20	kJ/mol	NIST Webbook
hvap	55.80	kJ/mol	NIST Webbook
hvap	53.20	kJ/mol	NIST Webbook
ie	8.30 ± 0.03	eV	NIST Webbook
ie	8.07	eV	NIST Webbook
ie	8.47 ± 0.05	eV	NIST Webbook
log10ws	-3.37		Crippen Method
logp	2.920		Crippen Method
mcvol	128.000	ml/mol	McGowan Method
pc	2870.00	kPa	KDB

rinpol	1154.00	NIST Webbook
rinpol	1109.00	NIST Webbook
rinpol	1109.00	NIST Webbook
rinpol	1109.00	NIST Webbook
rinpol	1109.00	NIST Webbook
rinpol	1110.00	NIST Webbook
rinpol	1099.50	NIST Webbook
rinpol	1104.00	NIST Webbook
rinpol	1110.00	NIST Webbook
rinpol	1118.00	NIST Webbook
rinpol	1125.00	NIST Webbook
rinpol	1108.40	NIST Webbook
rinpol	1111.40	NIST Webbook
rinpol	1110.50	NIST Webbook
rinpol	1117.50	NIST Webbook
rinpol	1125.00	NIST Webbook
rinpol	1108.00	NIST Webbook
rinpol	1108.40	NIST Webbook
rinpol	1111.40	NIST Webbook
rinpol	1113.00	NIST Webbook
rinpol	1105.05	NIST Webbook
rinpol	1137.00	NIST Webbook
rinpol	1140.00	NIST Webbook
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rinpol	1139.00	NIST Webbook
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rinpol	1149.00	NIST Webbook
rinpol	1150.00	NIST Webbook
rinpol	1097.70	NIST Webbook
rinpol	1151.00	NIST Webbook
rinpol	1123.00	NIST Webbook
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rinpol	1103.00	NIST Webbook
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rinpol	1104.00	NIST Webbook
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rinpol	1129.00	NIST Webbook
rinpol	1096.00	NIST Webbook
rinpol	1110.00	NIST Webbook
rinpol	1125.00	NIST Webbook
rinpol	1105.05	NIST Webbook
rinpol	1144.00	NIST Webbook
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rinpol	1108.80	NIST Webbook

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rinpol	1137.00		NIST Webbook
rinpol	1129.00		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1122.00		NIST Webbook
ripol	1456.30		NIST Webbook
ripol	1455.80		NIST Webbook
ripol	1430.00		NIST Webbook
ripol	1447.00		NIST Webbook
ripol	1441.00		NIST Webbook
ripol	1443.00		NIST Webbook
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ripol	1416.00		NIST Webbook
ripol	1422.00		NIST Webbook
ripol	1456.30		NIST Webbook
ripol	1455.80		NIST Webbook
ripol	1416.50		NIST Webbook
ripol	1474.50		NIST Webbook
ripol	1395.00		NIST Webbook
ripol	1410.50		NIST Webbook
sl	310.00	J/mol×K	NIST Webbook
tb	471.30	K	KDB
tc	679.00	K	KDB
tf	249.34 ± 0.20	K	NIST Webbook
tf	248.94 ± 0.40	K	NIST Webbook
tf	249.95 ± 0.20	K	NIST Webbook
tf	249.03 ± 0.50	K	NIST Webbook
tf	249.30 ± 0.30	K	NIST Webbook
tf	245.78 ± 0.50	K	NIST Webbook
tf	249.20 ± 1.00	K	NIST Webbook
tf	249.00 ± 0.20	K	NIST Webbook
tf	249.42 ± 0.03	K	NIST Webbook
tf	249.04 ± 0.30	K	NIST Webbook
tf	249.00	K	KDB
tf	249.46 ± 0.01	K	NIST Webbook
tf	249.45 ± 0.02	K	NIST Webbook
tf	249.38 ± 0.20	K	NIST Webbook
tt	248.60 ± 0.30	K	NIST Webbook
vc	0.487	m3/kmol	KDB
zc	0.2478280		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.77	J/mol×K	469.82	Joback Method
cpg	332.37	J/mol×K	678.39	Joback Method
cpg	321.58	J/mol×K	643.63	Joback Method
cpg	310.23	J/mol×K	608.87	Joback Method
cpg	298.28	J/mol×K	574.11	Joback Method
cpg	285.73	J/mol×K	539.34	Joback Method
cpg	272.57	J/mol×K	504.58	Joback Method
cpl	240.20	J/mol×K	297.10	NIST Webbook
dvisc	0.0007720	Pa×s	300.34	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
dvisc	0.0012469	Pa×s	266.44	Joback Method
dvisc	0.0005268	Pa×s	334.23	Joback Method
dvisc	0.0001983	Pa×s	469.82	Joback Method
hfust	12.93	kJ/mol	248.60	NIST Webbook
hfust	12.93	kJ/mol	248.60	NIST Webbook
hvapt	58.90	kJ/mol	392.50	NIST Webbook
hvapt	50.00	kJ/mol	425.00	NIST Webbook
hvapt	43.81	kJ/mol	471.30	KDB
rfi	1.51070		298.15	KDB
rhol	890.00	kg/m3	293.00	KDB
srf	0.03	N/m	298.20	KDB

Sources

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/mol685.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C527537&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=685

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

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid 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
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
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility