Benzene, 1-ethenyl-4-methyl-

Other names:	1-Ethenyl-4-methylbenzene
	1-METHYL-4-ETHENYLBENZENE
	1-Methyl-4-vinylbenzene
	1-p-Tolylethene
	4-METHYLSTYRENE
	4-Vinyltoluene
	P-VINYLTOLUENE
	Styrene, p-methyl-
	p-Methylstyrene
	para-Methylstyrene
Inchi:	InChI=1S/C9H10/c1-3-9-6-4-8(2)5-7-9/h3-7H,1H2,2H3
InchiKey:	JLBJTVDPSNHSKJ-UHFFFAOYSA-N
Formula:	C9H10
SMILES:	C=Cc1ccc(C)cc1
Mol. weight [g/mol]:	118.18
CAS:	622-97-9

Physical Properties

Property code	Value	Unit	Source
af	0.3250		KDB
affp	861.70	kJ/mol	NIST Webbook
basg	832.80	kJ/mol	NIST Webbook
gf	215.52	kJ/mol	Joback Method
hcg	5042.56	kJ/mol	KDB
hcn	4822.897	kJ/mol	KDB
hf	121.40	kJ/mol	Joback Method
hfus	11.44	kJ/mol	Joback Method
hvap	37.90	kJ/mol	Joback Method
ie	8.20	eV	NIST Webbook
ie	8.10 ± 0.10	eV	NIST Webbook
log10ws	-2.77		Crippen Method
logp	2.638		Crippen Method
mcvol	109.610	ml/mol	McGowan Method
pc	3370.00	kPa	KDB
rinpol	980.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	155.70		NIST Webbook

rinpol	982.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	977.50		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	155.70		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	979.00		NIST Webbook
rinpol	980.50		NIST Webbook
rinpol	965.90		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	978.60		NIST Webbook
rinpol	980.30		NIST Webbook
rinpol	978.60		NIST Webbook
rinpol	980.30		NIST Webbook
rinpol	977.50		NIST Webbook
rinpol	977.60		NIST Webbook
rinpol	977.90		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	158.68		NIST Webbook
ripol	1348.60		NIST Webbook
ripol	1396.80		NIST Webbook
ripol	1385.20		NIST Webbook
ripol	1349.00		NIST Webbook
ripol	1349.00		NIST Webbook
tb	444.65 ± 3.00	K	NIST Webbook
tb	445.65 ± 4.00	K	NIST Webbook
tb	446.00	K	NIST Webbook
tb	444.95 ± 2.00	K	NIST Webbook
tb	442.20	K	KDB
tc	659.70	K	KDB
tf	239.00 ± 0.15	K	NIST Webbook
tf	235.35 ± 0.50	K	NIST Webbook
tf	202.85	K	NIST Webbook
tf	239.30 ± 0.40	K	NIST Webbook
tf	239.00	K	KDB
vc	0.412	m3/kmol	KDB
zc	0.2534370		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.56	J/mol×K	646.99	Joback Method
cpg	199.98	J/mol×K	433.66	Joback Method
cpg	212.82	J/mol×K	469.22	Joback Method
cpg	224.92	J/mol×K	504.77	Joback Method
cpg	236.32	J/mol×K	540.33	Joback Method
cpg	247.04	J/mol×K	575.88	Joback Method
cpg	257.10	J/mol×K	611.44	Joback Method
dvisc	0.0002171	Pa×s	433.66	Joback Method
dvisc	0.0020152	Pa×s	228.37	Joback Method
dvisc	0.0010913	Pa×s	262.58	Joback Method
dvisc	0.0006808	Pa×s	296.80	Joback Method
dvisc	0.0004682	Pa×s	331.01	Joback Method
dvisc	0.0003454	Pa×s	365.23	Joback Method
dvisc	0.0002684	Pa×s	399.44	Joback Method
hvapt	47.60	kJ/mol	347.00	NIST Webbook
hvapt	35.98	kJ/mol	442.20	KDB
rfi	1.53950		298.15	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/mol724.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C622979&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=724

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

Legend

af: Acentric Factor

affp: Proton affinity

basg:	Gas basicity
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hcg:	Heat of Combustion, Gross form
hcn:	Heat of Combustion, Net Form
hf:	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
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
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