Benzene, 1-ethenyl-3-methyl-

Other names:	1-METHYL-3-ETHENYLBENZENE
	1-Methyl-3-vinylbenzene
	3-METHYLSTYRENE
	3-Vinyltoluene
	M-VINYLTOLUENE
	Styrene, m-methyl-
	m-Methylstyrene
Inchi:	InChI=1S/C9H10/c1-3-9-6-4-5-8(2)7-9/h3-7H,1H2,2H3
InchiKey:	JZHGRUMIRATHIU-UHFFFAOYSA-N
Formula:	C9H10
SMILES:	C=Cc1cccc(C)c1
Mol. weight [g/mol]:	118.18
CAS:	100-80-1

Physical Properties

Property code	Value	Unit	Source
af	0.3250		KDB
affp	849.40	kJ/mol	NIST Webbook
basg	820.50	kJ/mol	NIST Webbook
gf	215.52	kJ/mol	Joback Method
hcg	5042.98	kJ/mol	KDB
hcn	4823.316	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	8.15 ± 0.02	eV	NIST Webbook
ie	8.37	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	978.70		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	956.00		NIST Webbook
rinpol	156.20		NIST Webbook
rinpol	973.00		NIST Webbook
rinpol	977.00		NIST Webbook

rinpol	960.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	991.40		NIST Webbook
rinpol	973.20		NIST Webbook
rinpol	972.70		NIST Webbook
rinpol	978.70		NIST Webbook
rinpol	976.30		NIST Webbook
rinpol	997.80		NIST Webbook
rinpol	991.40		NIST Webbook
rinpol	973.20		NIST Webbook
rinpol	956.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	960.50		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	985.90		NIST Webbook
rinpol	976.30		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	973.20		NIST Webbook
ripol	1385.20		NIST Webbook
ripol	1396.80		NIST Webbook
ripol	1348.10		NIST Webbook
ripol	1388.10		NIST Webbook
ripol	1387.40		NIST Webbook
ripol	1348.00		NIST Webbook
ripol	1348.00		NIST Webbook
ripol	1385.20		NIST Webbook
tb	444.80	K	NIST Webbook
tb	442.65 ± 2.00	K	NIST Webbook
tb	437.15 ± 5.00	K	NIST Webbook
tb	441.20	K	KDB
tb	443.70	K	NIST Webbook
tc	658.20	K	KDB
tf	187.00	K	KDB
tf	203.00 ± 6.00	K	NIST Webbook
tf	186.81 ± 0.16	K	NIST Webbook
tt	250.78 ± 0.02	K	NIST Webbook
vc	0.412	m3/kmol	KDB
zc	0.2540150		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	47.50	kJ/mol	349.50	NIST Webbook
hvapt	36.36	kJ/mol	441.20	KDB
rfi	1.53850		298.15	KDB

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	334.70	K	2.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47415e+01
Coeff. B	-4.03605e+03
Coeff. C	-4.50060e+01
Temperature range (K), min.	324.24

Temperature range (K), max.	473.01

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.00504e+01
Coeff. B	-7.60691e+03
Coeff. C	-6.31787e+00
Coeff. D	1.26334e-06
Temperature range (K), min.	186.81
Temperature range (K), max.	657.00

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol723.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100801&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=723
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

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
pvap:	Vapor pressure
rfi:	Refractive Index
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility