Benzene, 1-ethenyl-2-methyl-

Other names:	1-Ethenyl-2-methylbenzene
	1-METHYL-2-ETHENYLBENZENE
	1-Methyl-2-vinylbenzene
	2-Ethenylmethylbenzene
	2-METHYLSTYRENE
	2-Methyl-1-vinylbenzene
	2-Vinyltoluene
	O-VINYLTOLUENE
	Styrene, o-methyl-
	o-Methylstyrene
Inchi:	InChI=1S/C9H10/c1-3-9-7-5-4-6-8(9)2/h3-7H,1H2,2H3
InchiKey:	NVZWEEGUWXZOKI-UHFFFAOYSA-N
Formula:	C9H10
SMILES:	C=Cc1ccccc1C
Mol. weight [g/mol]:	118.18
CAS:	611-15-4

Physical Properties

Property code	Value	Unit	Source
af	0.3250		KDB
affp	855.20	kJ/mol	NIST Webbook
basg	826.30	kJ/mol	NIST Webbook
gf	215.52	kJ/mol	Joback Method
hcg	5044.65	kJ/mol	KDB
hcn	4824.989	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 ± 0.02	eV	NIST Webbook
ie	8.53	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	974.20		NIST Webbook
rinpol	977.50		NIST Webbook
rinpol	1000.00		NIST Webbook

rinpol	982.00		NIST Webbook
rinpol	972.10		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	987.50		NIST Webbook
rinpol	993.20		NIST Webbook
rinpol	1000.40		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	990.60		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	1016.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	161.30		NIST Webbook
rinpol	155.50		NIST Webbook
rinpol	163.20		NIST Webbook
rinpol	955.00		NIST Webbook
rinpol	955.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	1000.40		NIST Webbook
rinpol	161.30		NIST Webbook
rinpol	147.84		NIST Webbook
rinpol	976.00		NIST Webbook
ripol	1342.00		NIST Webbook
ripol	1342.20		NIST Webbook
ripol	1327.00		NIST Webbook
ripol	1327.00		NIST Webbook
ripol	1342.00		NIST Webbook
tb	444.20	K	KDB
tb	433.15 ± 6.00	K	NIST Webbook
tc	662.70	K	KDB
tf	204.58 ± 0.10	K	NIST Webbook
tf	205.00	K	KDB
tf	204.76 ± 0.50	K	NIST Webbook
vc	0.412	m3/kmol	KDB
zc	0.2522900		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	257.10	J/mol×K	611.44	Joback Method
cpg	236.32	J/mol×K	540.33	Joback Method
cpg	224.92	J/mol×K	504.77	Joback Method
cpg	212.82	J/mol×K	469.22	Joback Method
cpg	199.98	J/mol×K	433.66	Joback Method
cpg	247.04	J/mol×K	575.88	Joback Method
cpg	266.56	J/mol×K	646.99	Joback Method
dvisc	0.0020152	Pa×s	228.37	Joback Method
dvisc	0.0002171	Pa×s	433.66	Joback Method
dvisc	0.0002684	Pa×s	399.44	Joback Method
dvisc	0.0003454	Pa×s	365.23	Joback Method
dvisc	0.0004682	Pa×s	331.01	Joback Method
dvisc	0.0006808	Pa×s	296.80	Joback Method
dvisc	0.0010913	Pa×s	262.58	Joback Method
hvapt	36.82	kJ/mol	444.20	KDB
hvapt	47.90	kJ/mol	345.00	NIST Webbook
rfi	1.54130		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53995e+01
Coeff. B	-4.08230e+03
Coeff. C	-5.44980e+01
Temperature range (K), min.	324.64
Temperature range (K), max.	459.17

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.28813e+01
Coeff. B	-8.58406e+03
Coeff. C	-9.80992e+00
Coeff. D	4.53627e-06
Temperature range (K), min.	204.58
Temperature range (K), max.	659.00

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=722
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/mol722.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C611154&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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