Benzene, 1-ethenyl-4-ethyl-

Other names:	1-ETHYL-4-ETHENYLBENZENE
	1-Ethenyl-4-ethylbenzene
	4-Ethenylstyrene
	4-Ethyl-1-ethenyl benzene
	4-Ethylstyrene
	Styrene, p-ethyl-
	p-Ethylstyrene
	p-Ethylvinylbenzene
Inchi:	InChI=1S/C10H12/c1-3-9-5-7-10(4-2)8-6-9/h3,5-8H,1,4H2,2H3
InchiKey:	WHFHDVDXYKOSKI-UHFFFAOYSA-N
Formula:	C10H12
SMILES:	C=Cc1ccc(CC)cc1
Mol. weight [g/mol]:	132.20
CAS:	3454-07-7

Physical Properties

Property code	Value	Unit	Source
gf	223.94	kJ/mol	Joback Method
hf	100.76	kJ/mol	Joback Method
hfus	14.03	kJ/mol	Joback Method
hvap	40.12	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.892		Crippen Method
mcvol	123.700	ml/mol	McGowan Method
pc	3018.96	kPa	Joback Method
rinpol	1073.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	179.40		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1071.70		NIST Webbook
rinpol	1071.70		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1072.00		NIST Webbook

rinpol	1073.20		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1073.00		NIST Webbook
ripol	1431.00		NIST Webbook
ripol	1431.00		NIST Webbook
ripol	1462.00		NIST Webbook
ripol	1482.70		NIST Webbook
ripol	1481.40		NIST Webbook
ripol	1481.40		NIST Webbook
ripol	1431.30		NIST Webbook
ripol	1455.00		NIST Webbook
tb	456.54	K	Joback Method
tc	667.08	K	Joback Method
tf	223.42 ± 0.50	K	NIST Webbook
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.59	J/mol×K	456.54	Joback Method
cpg	254.60	J/mol×K	491.63	Joback Method
cpg	267.82	J/mol×K	526.72	Joback Method
cpg	280.28	J/mol×K	561.81	Joback Method
cpg	292.01	J/mol×K	596.90	Joback Method
cpg	303.05	J/mol×K	631.99	Joback Method
cpg	313.43	J/mol×K	667.08	Joback Method
dvisc	0.0021934	Pa×s	239.64	Joback Method
dvisc	0.0011572	Pa×s	275.79	Joback Method
dvisc	0.0007081	Pa×s	311.94	Joback Method
dvisc	0.0004798	Pa×s	348.09	Joback Method
dvisc	0.0003498	Pa×s	384.24	Joback Method
dvisc	0.0002693	Pa×s	420.39	Joback Method
dvisc	0.0002161	Pa×s	456.54	Joback Method
hvapt	48.40	kJ/mol	394.50	NIST Webbook

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45697e+01
Coeff. B	-3.89779e+03
Coeff. C	-7.05450e+01
Temperature range (K), min.	343.46
Temperature range (K), max.	491.55

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.23831e+02
Coeff. B	-1.06224e+04
Coeff. C	-1.60451e+01
Coeff. D	9.99062e-06
Temperature range (K), min.	341.15
Temperature range (K), max.	448.15

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=742

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/mol742.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3454077&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
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