Benzene, 1-ethenyl-3-ethyl-

Other names:	1-ETHYL-3-ETHENYLBENZENE
	1-Ethenyl-3-ethylbenzene
	1-Ethyl-3-vinylbenzene
	1-Vinyl-3-ethylbenzene
	3-Ethyl-1-ethenyl benzene
	3-Ethylstyrene
	3-Vinylethylbenzene
	Styrene, m-ethyl-
	m-Ethyl vinylbenzen
	m-Ethylstyrene
	m-Ethylvinylbenzene
	m-Vinylethylbenzene
Inchi:	InChI=1S/C10H12/c1-3-9-6-5-7-10(4-2)8-9/h3,5-8H,1,4H2,2H3
InchiKey:	XHUZSRRCICJJCN-UHFFFAOYSA-N
Formula:	C10H12
SMILES:	C=Cc1cccc(CC)c1
Mol. weight [g/mol]:	132.20
CAS:	7525-62-4

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	1066.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1065.80		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1063.90		NIST Webbook
rinpol	1064.40		NIST Webbook

rinpol	1066.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	178.30		NIST Webbook
rinpol	180.10		NIST Webbook
rinpol	1063.90		NIST Webbook
rinpol	1074.00		NIST Webbook
ripol	1423.70		NIST Webbook
ripol	1424.00		NIST Webbook
tb	456.54	K	Joback Method
tc	667.08	K	Joback Method
tf	171.85 ± 0.60	K	NIST Webbook
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.43	J/mol×K	667.08	Joback Method
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
dvisc	0.0002161	Pa×s	456.54	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
hvapt	49.60	kJ/mol	398.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41861e+01

Coeff. B	-3.77678e+03
Coeff. C	-6.99200e+01
Temperature range (K), min.	341.66
Temperature range (K), max.	495.49

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.24616e+02
Coeff. B	-1.08113e+04
Coeff. C	-1.60909e+01
Coeff. D	9.83659e-06
Temperature range (K), min.	343.15
Temperature range (K), max.	453.15

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7525624&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=741

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/mol741.mol

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