Benzene, 2-ethenyl-1,3-dimethyl-

Other names:	1,3-DIMETHYL-2-ETHENYLBENZENE
	1,3-DIMETHYL-2-VINYLBENZENE
	2,6-DIMETHYLSTYRENE
	Styrene, 2,6-dimethyl-
Inchi:	InChI=1S/C10H12/c1-4-10-8(2)6-5-7-9(10)3/h4-7H,1H2,2-3H3
InchiKey:	OWRKXOZFTROHSH-UHFFFAOYSA-N
Formula:	C10H12
SMILES:	C=Cc1c(C)cccc1C
Mol. weight [g/mol]:	132.20
CAS:	2039-90-9

Physical Properties

Property code	Value	Unit	Source
gf	214.31	kJ/mol	Joback Method
hf	89.29	kJ/mol	Joback Method
hfus	13.64	kJ/mol	Joback Method
hvap	40.78	kJ/mol	Joback Method
ie	8.48	eV	NIST Webbook
ie	8.10 ± 0.02	eV	NIST Webbook
log10ws	-3.25		Crippen Method
logp	2.946		Crippen Method
mcvol	123.700	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
rinpol	1070.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1117.90		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1078.00		NIST Webbook
tb	461.52	K	Joback Method
tc	673.43	K	Joback Method
tf	234.50 ± 0.40	K	NIST Webbook
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.30	J/mol×K	461.52	Joback Method
cpg	302.08	J/mol×K	638.11	Joback Method
cpg	291.26	J/mol×K	602.79	Joback Method
cpg	279.80	J/mol×K	567.47	Joback Method
cpg	267.67	J/mol×K	532.16	Joback Method
cpg	254.85	J/mol×K	496.84	Joback Method
cpg	312.28	J/mol×K	673.43	Joback Method
dvisc	0.0002066	Pa×s	461.52	Joback Method
dvisc	0.0002519	Pa×s	426.63	Joback Method
dvisc	0.0003181	Pa×s	391.73	Joback Method
dvisc	0.0004204	Pa×s	356.84	Joback Method
dvisc	0.0005904	Pa×s	321.95	Joback Method
dvisc	0.0009004	Pa×s	287.05	Joback Method
dvisc	0.0015433	Pa×s	252.16	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	339.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45622e+01
Coeff. B	-3.89523e+03
Coeff. C	-7.05780e+01
Temperature range (K), min.	343.46
Temperature range (K), max.	491.65

Sources

KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=745
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2039909&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume