

# Benzene, 2-ethenyl-1,4-dimethyl-

<b>Other names:</b>	1,4-DIMETHYL-2-ETHENYLBENZENE 1,4-DIMETHYL-2-VINYLBENZENE 2,5-DIMETHYLSTYRENE Styrene, 2,5-dimethyl-
<b>Inchi:</b>	InChI=1S/C10H12/c1-4-10-7-8(2)5-6-9(10)3/h4-7H,1H2,2-3H3
<b>InchiKey:</b>	DBWWINQJTZYDFK-UHFFFAOYSA-N
<b>Formula:</b>	C10H12
<b>SMILES:</b>	<chem>C=Cc1cc(C)ccc1C</chem>
<b>Mol. weight [g/mol]:</b>	132.20
<b>CAS:</b>	2039-89-6

## 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	8.00 ± 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	1079.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1078.70		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1075.80		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1089.00		NIST Webbook
rinpol	1066.00		NIST Webbook

rinpol	1067.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1101.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	180.10		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	180.10		NIST Webbook
rinpol	1059.00		NIST Webbook
ripol	1444.00		NIST Webbook
ripol	1459.00		NIST Webbook
ripol	1432.20		NIST Webbook
ripol	1444.00		NIST Webbook
ripol	1432.00		NIST Webbook
ripol	1425.00		NIST Webbook
ripol	1434.00		NIST Webbook
ripol	1432.20		NIST Webbook
tb	461.52	K	Joback Method
tc	673.43	K	Joback Method
tf	238.00 ± 0.40	K	NIST Webbook
vc	0.469	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.28	J/mol×K	673.43	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	241.30	J/mol×K	461.52	Joback Method
dvisc	0.0015433	Paxs	252.16	Joback Method
dvisc	0.0002066	Paxs	461.52	Joback Method
dvisc	0.0002519	Paxs	426.63	Joback Method

dvisc	0.0003181	Paxs	391.73	Joback Method
dvisc	0.0004204	Paxs	356.84	Joback Method
dvisc	0.0005904	Paxs	321.95	Joback Method
dvisc	0.0009004	Paxs	287.05	Joback Method
hvapt	48.10	kJ/mol	377.50	NIST Webbook

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	344.70	K	1.30	NIST Webbook
tbrp	342.20	K	1.30	NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>KDB:</b>	<a href="https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=748">https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=748</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2039896&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2039896&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure

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

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