

# 1,4-Pentadiene, 3-ethenyl-

<b>Other names:</b>	1,4-Pentadiene, 3-vinyl- (CH <sub>2</sub> =CH) <sub>3</sub> CH
<b>Inchi:</b>	InChI=1S/C7H10/c1-4-7(5-2)6-3/h4-7H,1-3H2
<b>InchiKey:</b>	HEKRPWJODWSOQV-UHFFFAOYSA-N
<b>Formula:</b>	C <sub>7</sub> H <sub>10</sub>
<b>SMILES:</b>	C=CC(C=C)C=C
<b>Mol. weight [g/mol]:</b>	94.15
<b>CAS:</b>	26456-63-3

## Physical Properties

Property code	Value	Unit	Source
gf	269.14	kJ/mol	Joback Method
hf	183.20	kJ/mol	Joback Method
hfus	6.52	kJ/mol	Joback Method
hvap	28.78	kJ/mol	Joback Method
ie	9.50	eV	NIST Webbook
ie	9.10	eV	NIST Webbook
log10ws	-2.07		Crippen Method
logp	2.161		Crippen Method
mcvol	96.590	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
tb	349.16	K	Joback Method
tc	527.46	K	Joback Method
tf	148.37	K	Joback Method
vc	0.364	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	153.48	J/mol×K	349.16	Joback Method
cpg	163.93	J/mol×K	378.88	Joback Method
cpg	173.87	J/mol×K	408.59	Joback Method
cpg	183.33	J/mol×K	438.31	Joback Method
cpg	192.31	J/mol×K	468.03	Joback Method

cpg	200.84	J/molxK	497.74	Joback Method
cpg	208.94	J/molxK	527.46	Joback Method
dvisc	0.0047915	Paxs	148.37	Joback Method
dvisc	0.0017502	Paxs	181.84	Joback Method
dvisc	0.0008744	Paxs	215.30	Joback Method
dvisc	0.0005265	Paxs	248.76	Joback Method
dvisc	0.0003575	Paxs	282.23	Joback Method
dvisc	0.0002636	Paxs	315.69	Joback Method
dvisc	0.0002060	Paxs	349.16	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C26456633&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C26456633&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>
<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>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>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>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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