1,3-Pentadiene, (E)-

Other names:	(E)-1,3-PENTADIENE
	(E)-CH2=CHCH=CHCH3
	1,trans-3-Pentadiene
	Pentadiene-1,3,trans
	TRANS-1,3-PENTADIENE
	TRANS-1-METHYLBUTADIENE
	TRANS-PIPERYLENE
	trans-penta-1,3-diene
Inchi:	InChI=1S/C5H8/c1-3-5-4-2/h3-5H,1H2,2H3/b5-4+
InchiKey:	PMJHHCWVYXUKFD-SNAWJCMRSA-N
Formula:	C5H8
SMILES:	C=CC=CC
Mol. weight [g/mol]:	68.12
CAS:	2004-70-8

Physical Properties

Property code	Value	Unit	Source
af	0.1750		KDB
affp	834.10	kJ/mol	NIST Webbook
basg	804.40	kJ/mol	NIST Webbook
chg	-3186.70 ± 0.63	kJ/mol	NIST Webbook
dm	0.70	debye	KDB
gf	146.80	kJ/mol	KDB
hcg	3158.71	kJ/mol	KDB
hcn	2982.690	kJ/mol	KDB
hf	75.77 ± 0.67	kJ/mol	NIST Webbook
hf	77.87	kJ/mol	KDB
hfus	7.63	kJ/mol	Joback Method
hvap	27.80	kJ/mol	NIST Webbook
ie	8.59 ± 0.02	eV	NIST Webbook
ie	8.56	eV	NIST Webbook
ie	8.61 ± 0.02	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
ie	8.61	eV	NIST Webbook
ie	8.59 ± 0.02	eV	NIST Webbook
log10ws	-1.62		Crippen Method
logp	1.748		Crippen Method

mcvol	72.710	ml/mol	McGowan Method
pc	3990.00	kPa	KDB
rinpol	515.00		NIST Webbook
rinpol	516.20		NIST Webbook
rinpol	526.00		NIST Webbook
rinpol	516.00		NIST Webbook
rinpol	513.75		NIST Webbook
rinpol	515.70		NIST Webbook
rinpol	516.00		NIST Webbook
rinpol	518.00		NIST Webbook
rinpol	516.50		NIST Webbook
rinpol	518.00		NIST Webbook
rinpol	528.00		NIST Webbook
rinpol	526.00		NIST Webbook
rinpol	524.00		NIST Webbook
rinpol	515.00		NIST Webbook
rinpol	521.00		NIST Webbook
rinpol	523.00		NIST Webbook
rinpol	519.00		NIST Webbook
rinpol	515.70		NIST Webbook
rinpol	528.00		NIST Webbook
rinpol	515.00		NIST Webbook
rinpol	528.00		NIST Webbook
rinpol	521.00		NIST Webbook
rinpol	515.80		NIST Webbook
rinpol	526.00		NIST Webbook
rinpol	518.00		NIST Webbook
rinpol	515.80		NIST Webbook
rinpol	521.00		NIST Webbook
rinpol	522.00		NIST Webbook
rinpol	506.00		NIST Webbook
rinpol	526.00		NIST Webbook
rinpol	515.00		NIST Webbook
rinpol	524.00		NIST Webbook
rinpol	519.00		NIST Webbook
rinpol	516.00		NIST Webbook
sg	315.60	J/mol×K	NIST Webbook
sl	227.11	J/mol×K	NIST Webbook
tb	315.20 ± 0.40	K	NIST Webbook
tb	315.32 ± 0.30	K	NIST Webbook
tb	314.70 ± 2.00	K	NIST Webbook
tb	315.20	K	NIST Webbook
tb	315.10	K	KDB
tb	315.00 ± 0.60	K	NIST Webbook

tb	315.00 ± 2.00	K	NIST Webbook
tb	315.00 ± 2.00	K	NIST Webbook
tc	496.00	K	KDB
tf	185.40 ± 0.02	K	NIST Webbook
tf	185.64 ± 0.05	K	NIST Webbook
tf	185.66 ± 0.03	K	NIST Webbook
tf	185.00 ± 0.30	K	NIST Webbook
tf	185.50 ± 0.50	K	NIST Webbook
tf	185.10 ± 0.50	K	NIST Webbook
tf	184.30 ± 0.50	K	NIST Webbook
tf	185.70	K	KDB
tt	185.71 ± 0.05	K	NIST Webbook
vc	0.275	m3/kmol	KDB
zc	0.2660650		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	116.31	J/mol×K	373.19	Joback Method
cpg	100.21	J/mol×K	314.64	Joback Method
cpg	123.76	J/mol×K	402.46	Joback Method
cpg	130.84	J/mol×K	431.74	Joback Method
cpg	137.57	J/mol×K	461.01	Joback Method
cpg	143.95	J/mol×K	490.29	Joback Method
cpg	108.47	J/mol×K	343.91	Joback Method
cpl	149.33	J/mol×K	298.15	NIST Webbook
dvisc	0.0001957	Pa×s	285.41	Joback Method
dvisc	0.0002581	Pa×s	256.18	Joback Method
dvisc	0.0003655	Pa×s	226.95	Joback Method
dvisc	0.0005737	Pa×s	197.73	Joback Method
dvisc	0.0001562	Pa×s	314.64	Joback Method
dvisc	0.0010531	Pa×s	168.50	Joback Method
dvisc	0.0024945	Pa×s	139.27	Joback Method
hfust	7.14	kJ/mol	185.70	NIST Webbook
hfust	7.14	kJ/mol	185.70	NIST Webbook
hfust	7.14	kJ/mol	185.71	NIST Webbook
hvapt	31.30	kJ/mol	227.50	NIST Webbook
hvapt	29.50	kJ/mol	290.00	NIST Webbook
hvapt	30.70	kJ/mol	242.00	NIST Webbook
hvapt	27.03	kJ/mol	317.20	KDB
hvapt	28.30	kJ/mol	304.00	NIST Webbook

rfi	1.42669		298.15	KDB
rhol	676.00	kg/m3	293.00	KDB
sfust	38.47	J/mol×K	185.71	NIST Webbook
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.34984e+01
Coeff. B	-2.39392e+03
Coeff. C	-4.55170e+01
Temperature range (K), min.	226.73
Temperature range (K), max.	337.92

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.28741e+01
Coeff. B	-4.98799e+03
Coeff. C	-5.68031e+00
Coeff. D	2.52732e-06
Temperature range (K), min.	185.71
Temperature range (K), max.	500.00

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2004708&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=361

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/research/kdb/hcprop/showprop.php?cmpid=361

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chg:	Standard gas enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hcg:	Heat of Combustion, Gross form
hcn:	Heat of Combustion, Net Form
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.