1,3-Pentadiene, (Z)-

Other names:	(Z)-1,3-PENTADIENE
	(Z)-CH2=CHCH=CHCH3
	(Z)-penta-1,3-diene
	1,cis-3-Pentadiene
	CIS-1,3-PENTADIENE
	CIS-1-METHYLBUTADIENE
	CIS-PIPERYLENE
	Pentadiene-1,3, cis-
Inchi:	InChI=1S/C5H8/c1-3-5-4-2/h3-5H,1H2,2H3/b5-4-
InchiKey:	PMJHHCWVYXUKFD-PLNGDYQASA-N
Formula:	C5H8
SMILES:	C=CC=CC
Mol. weight [g/mol]:	68.12
CAS:	1574-41-0

Physical Properties

Property code	Value	Unit	Source
chg	-3193.60 ± 0.88	kJ/mol	NIST Webbook
gf	159.28	kJ/mol	Joback Method
hf	82.72 ± 0.92	kJ/mol	NIST Webbook
hfus	7.63	kJ/mol	Joback Method
hvap	28.30	kJ/mol	NIST Webbook
ie	8.64	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
ie	8.67 ± 0.02	eV	NIST Webbook
ie	8.63	eV	NIST Webbook
ie	8.59	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
ie	8.62 ± 0.03	eV	NIST Webbook
log10ws	-1.62		Crippen Method
logp	1.748		Crippen Method
mcvol	72.710	ml/mol	McGowan Method
pc	3886.79	kPa	Joback Method
rinpol	522.80		NIST Webbook
rinpol	527.00		NIST Webbook
rinpol	525.00		NIST Webbook
rinpol	524.00		NIST Webbook

rinpol	527.00		NIST Webbook
rinpol	541.20		NIST Webbook
rinpol	510.50		NIST Webbook
rinpol	536.00		NIST Webbook
rinpol	524.00		NIST Webbook
rinpol	536.00		NIST Webbook
rinpol	532.00		NIST Webbook
rinpol	536.00		NIST Webbook
rinpol	524.00		NIST Webbook
rinpol	537.00		NIST Webbook
rinpol	510.00		NIST Webbook
rinpol	525.00		NIST Webbook
rinpol	524.80		NIST Webbook
rinpol	524.40		NIST Webbook
rinpol	525.10		NIST Webbook
rinpol	536.10		NIST Webbook
rinpol	536.00		NIST Webbook
sg	322.80	J/mol×K	NIST Webbook
sl	233.25	J/mol×K	NIST Webbook
tb	317.30	K	NIST Webbook
tb	317.18 ± 0.40	K	NIST Webbook
tb	316.65 ± 1.00	K	NIST Webbook
tb	316.00 ± 2.00	K	NIST Webbook
tb	317.20 ± 0.40	K	NIST Webbook
tc	490.29	K	Joback Method
tf	132.33 ± 0.02	K	NIST Webbook
tf	132.31	K	KDB
tf	132.31 ± 0.04	K	NIST Webbook
tf	132.31 ± 0.03	K	NIST Webbook
tf	131.57 ± 0.50	K	NIST Webbook
tt	132.35 ± 0.05	K	NIST Webbook
vc	0.277	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	143.95	J/mol×K	490.29	Joback Method
cpg	116.31	J/mol×K	373.19	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	100.21	J/mol×K	314.64	Joback Method
cpg	108.47	J/mol×K	343.91	Joback Method
cpl	146.57	J/mol×K	298.15	NIST Webbook
dvisc	0.0001562	Pa×s	314.64	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	0.0010531	Pa×s	168.50	Joback Method
dvisc	0.0001957	Pa×s	285.41	Joback Method
dvisc	0.0024945	Pa×s	139.27	Joback Method
hfust	5.64	kJ/mol	132.35	NIST Webbook
hfust	5.64	kJ/mol	132.40	NIST Webbook
hfust	5.64	kJ/mol	132.40	NIST Webbook
hvapt	28.80	kJ/mol	303.50	NIST Webbook
hvapt	31.90	kJ/mol	227.50	NIST Webbook
hvapt	30.10	kJ/mol	290.50	NIST Webbook
hvapt	31.20	kJ/mol	242.50	NIST Webbook
sfust	42.60	J/mol×K	132.35	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37915e+01
Coeff. B	-2.57592e+03
Coeff. C	-3.64890e+01
Temperature range (K), min.	227.24
Temperature range (K), max.	340.25

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.03742e+01
Coeff. B	-5.30049e+03
Coeff. C	-6.85336e+00
Coeff. D	4.24873e-06
Temperature range (K), min.	132.35
Temperature range (K), max.	499.00

Sources

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=360
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=360
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1574410&Units=SI

Legend

chg:	Standard gas enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

vc: Critical Volume