1,2-Pentadiene

Other names:	1-METHYL-2,3-BUTADIENE
	CH2=C=CHCH2CH3
	ETHYLALLENE
	penta-1,2-diene
Inchi:	InChI=1S/C5H8/c1-3-5-4-2/h5H,1,4H2,2H3
InchiKey:	LVMTVPFRTKXRPH-UHFFFAOYSA-N
Formula:	C5H8
SMILES:	C=C=CCC
Mol. weight [g/mol]:	68.12
CAS:	591-95-7

Physical Properties

Property code	Value	Unit	Source
af	0.1730		KDB
chg	-3251.60 ± 0.63	kJ/mol	NIST Webbook
gf	210.60	kJ/mol	KDB
hcg	3222.77	kJ/mol	KDB
hcn	3046.705	kJ/mol	KDB
hf	145.70	kJ/mol	KDB
hf	140.60 ± 0.67	kJ/mol	NIST Webbook
hfus	9.56	kJ/mol	Joback Method
hvap	28.70	kJ/mol	NIST Webbook
ie	9.42	eV	NIST Webbook
ie	9.25 ± 0.02	eV	NIST Webbook
ie	9.22	eV	NIST Webbook
log10ws	-1.64		Crippen Method
logp	1.737		Crippen Method
mcvol	72.710	ml/mol	McGowan Method
pc	4070.00	kPa	KDB
rinpol	527.00		NIST Webbook
rinpol	527.00		NIST Webbook
rinpol	526.00		NIST Webbook
rinpol	526.00		NIST Webbook
rinpol	526.00		NIST Webbook
rinpol	526.00		NIST Webbook
rinpol	527.00		NIST Webbook
rinpol	525.00		NIST Webbook

rinpol	527.00		NIST Webbook
rinpol	526.00		NIST Webbook
rinpol	526.00		NIST Webbook
sg	334.80	J/mol×K	NIST Webbook
sl	244.97	J/mol×K	NIST Webbook
tb	318.00	K	KDB
tb	318.10 ± 0.40	K	NIST Webbook
tb	319.00 ± 2.00	K	NIST Webbook
tb	318.00 ± 1.00	K	NIST Webbook
tc	503.00	K	KDB
tf	135.88 ± 0.03	K	NIST Webbook
tf	135.90	K	KDB
tf	135.82 ± 0.04	K	NIST Webbook
tf	135.84 ± 0.03	K	NIST Webbook
tf	135.89 ± 0.02	K	NIST Webbook
tf	135.87 ± 0.04	K	NIST Webbook
tt	135.89 ± 0.05	K	NIST Webbook
vc	0.276	m3/kmol	KDB
zc	0.2685960		KDB
zra	0.27		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	141.68	J/mol×K	462.02	Joback Method
cpg	109.06	J/mol×K	313.75	Joback Method
cpg	115.97	J/mol×K	343.40	Joback Method
cpg	122.69	J/mol×K	373.06	Joback Method
cpg	129.22	J/mol×K	402.71	Joback Method
cpg	135.54	J/mol×K	432.36	Joback Method
cpg	147.61	J/mol×K	491.67	Joback Method
cpl	150.83	J/mol×K	298.15	NIST Webbook
hfust	7.56	kJ/mol	135.90	NIST Webbook
hfust	7.56	kJ/mol	135.89	NIST Webbook
hfust	7.56	kJ/mol	135.90	NIST Webbook
hvapt	29.10	kJ/mol	302.00	NIST Webbook
hvapt	27.57	kJ/mol	318.00	KDB
hvapt	31.60	kJ/mol	240.00	NIST Webbook
hvapt	30.60	kJ/mol	290.00	NIST Webbook
hvapt	32.20	kJ/mol	229.00	NIST Webbook
rfi	1.41773		298.15	KDB

rhol	693.00	kg/m3	293.00	KDB
sfust	55.63	J/mol×K	135.89	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	1.38337e+01
Coeff. B	-2.59213e+03
Coeff. C	-3.68150e+01
Temperature range (K), min.	228.17
Temperature range (K), max.	340.98

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C591957&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

KDB: https://www.cheric.org/files/research/kdb/mol/mol359.mol

Legend

af: Acentric Factor

chg: Standard gas enthalpy of combustion

cpg: Ideal gas heat capacity

cpl: Liquid phase heat capacity

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
zra:	Rackett Parameter