1,4-Pentadiene

Other names:	CH2=CHCH2CH=CH2
	PENTA-1,4-DIENE
	Pentadiene-1,4
Inchi:	InChI=1S/C5H8/c1-3-5-4-2/h3-4H,1-2,5H2
InchiKey:	QYZLKGVUSQXAMU-UHFFFAOYSA-N
Formula:	C5H8
SMILES:	C=CCC=C
Mol. weight [g/mol]:	68.12
CAS:	591-93-5

Physical Properties

Property code	Value	Unit	Source
af	0.1040		KDB
chg	-3217.20 ± 1.30	kJ/mol	NIST Webbook
dm	0.40	debye	KDB
gf	170.40	kJ/mol	KDB
hcg	3191.72	kJ/mol	KDB
hcn	3015.660	kJ/mol	KDB
hf	106.30 ± 1.30	kJ/mol	NIST Webbook
hf	105.50	kJ/mol	KDB
hfus	6.15	kJ/mol	Joback Method
hvap	25.20	kJ/mol	NIST Webbook
ie	9.62 ± 0.02	eV	NIST Webbook
ie	9.46	eV	NIST Webbook
ie	9.72	eV	NIST Webbook
ie	9.62 ± 0.02	eV	NIST Webbook
ie	9.58	eV	NIST Webbook
ie	7.97	eV	NIST Webbook
log10ws	-2.09		Estimated Solubility Method
log10ws	-2.09		Aqueous Solubility Prediction Method
logp	1.748		Crippen Method
mcvol	72.710	ml/mol	McGowan Method
pc	3790.00	kPa	KDB
rinpol	464.30		NIST Webbook
rinpol	465.00		NIST Webbook
rinpol	465.00		NIST Webbook

rinpol	471.00		NIST Webbook
rinpol	480.50		NIST Webbook
rinpol	462.50		NIST Webbook
rinpol	480.00		NIST Webbook
rinpol	480.50		NIST Webbook
rinpol	464.00		NIST Webbook
rinpol	462.20		NIST Webbook
rinpol	480.00		NIST Webbook
rinpol	461.00		NIST Webbook
rinpol	463.00		NIST Webbook
rinpol	479.00		NIST Webbook
rinpol	463.00		NIST Webbook
rinpol	463.80		NIST Webbook
rinpol	462.11		NIST Webbook
rinpol	480.00		NIST Webbook
rinpol	464.30		NIST Webbook
ripol	646.00		NIST Webbook
ripol	646.00		NIST Webbook
sg	333.97	J/mol×K	NIST Webbook
sl	248.86	J/mol×K	NIST Webbook
sl	338.70	J/mol×K	NIST Webbook
tb	299.10	K	KDB
tc	478.00	K	KDB
tf	124.90	K	KDB
tf	124.88	K	Aqueous Solubility Prediction Method
tt	124.91 ± 0.05	K	NIST Webbook
tt	124.30 ± 0.20	K	NIST Webbook
vc	0.276	m3/kmol	KDB
zc	0.2631990		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.50	J/mol×K	448.40	Joback Method
cpg	101.81	J/mol×K	307.16	Joback Method
cpg	109.60	J/mol×K	335.41	Joback Method
cpg	117.05	J/mol×K	363.66	Joback Method
cpg	124.18	J/mol×K	391.90	Joback Method
cpg	130.99	J/mol×K	420.15	Joback Method
cpg	143.72	J/mol×K	476.65	Joback Method

cpl	146.61	J/mol×K	292.50	NIST Webbook
cpl	146.82	J/mol×K	298.15	NIST Webbook
dvisc	0.0002853	Pa×s	252.30	Joback Method
dvisc	0.0003909	Pa×s	224.88	Joback Method
dvisc	0.0005843	Pa×s	197.45	Joback Method
dvisc	0.0009946	Pa×s	170.02	Joback Method
dvisc	0.0001800	Pa×s	307.16	Joback Method
dvisc	0.0002216	Pa×s	279.73	Joback Method
dvisc	0.0020771	Pa×s	142.59	Joback Method
hfust	6.14	kJ/mol	124.30	NIST Webbook
hfust	6.14	kJ/mol	124.30	NIST Webbook
hfust	6.14	kJ/mol	124.30	NIST Webbook
hfust	6.07	kJ/mol	124.90	NIST Webbook
hvapt	28.10	kJ/mol	271.50	NIST Webbook
hvapt	29.30	kJ/mol	221.50	NIST Webbook
hvapt	27.03	kJ/mol	299.10	KDB
hvapt	29.10	kJ/mol	226.00	NIST Webbook
hvapt	28.40	kJ/mol	224.50	NIST Webbook
hvapt	26.50	kJ/mol	294.00	NIST Webbook
rfi	1.38542		298.15	KDB
rhol	661.00	kg/m3	293.00	KDB
sfust	48.62	J/mol×K	124.90	NIST Webbook
sfust	49.41	J/mol×K	124.30	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	1.33916e+01
Coeff. B	-2.25302e+03
Coeff. C	-4.21950e+01
Temperature range (K), min.	214.13
Temperature range (K), max.	321.03

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.26109e+01

Coeff. B	-4.72040e+03
Coeff. C	-5.69053e+00
Coeff. D	2.57602e-06
Temperature range (K), min.	124.86
Temperature range (K), max.	479.00

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=362
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB:	https://www.cheric.org/files/research/kdb/mol/mol362.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C591935&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ripol:	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