1,5-Hexadiene

Other names:	.alpha.,.omega.-hexadiene
	BIALLYL
	CH2=CHCH2CH2CH=CH2
	Diallyl
	HEXADIENE
	Hexa-1,5-diene
	«alpha»,«OMEGA»-Hexadiene
	Â«alphaÂ»,Â«OMEGAÂ»-Hexadiene
Inchi:	InChI=1S/C6H10/c1-3-5-6-4-2/h3-4H,1-2,5-6H2
InchiKey:	PYGSKMBEVAICCR-UHFFFAOYSA-N
Formula:	C6H10
SMILES:	C=CCCC=C
Mol. weight [g/mol]:	82.14
CAS:	592-42-7

Physical Properties

Property code	Value	Unit	Source
af	0.1600		KDB
chl	-3844.30 ± 0.30	kJ/mol	NIST Webbook
chl	-3881.00	kJ/mol	NIST Webbook
chs	-3874.00	kJ/mol	NIST Webbook
gf	175.32	kJ/mol	Joback Method
hcg	3849.28	kJ/mol	KDB
hcn	3629.202	kJ/mol	KDB
hf	85.00 ± 2.00	kJ/mol	NIST Webbook
hf	83.74	kJ/mol	KDB
hfus	8.74	kJ/mol	Joback Method
hvap	27.61	kJ/mol	Joback Method
ie	9.29 ± 0.05	eV	NIST Webbook
ie	9.27 ± 0.05	eV	NIST Webbook
ie	9.25	eV	NIST Webbook
ie	9.59 ± 0.02	eV	NIST Webbook
ie	9.29	eV	NIST Webbook
log10ws	-2.68		Aqueous Solubility Prediction Method
log10ws	-2.68		Estimated Solubility Method

logp	2.139		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	3440.00	kPa	KDB
rinpol	564.00		NIST Webbook
rinpol	563.00		NIST Webbook
rinpol	564.00		NIST Webbook
rinpol	566.00		NIST Webbook
rinpol	566.00		NIST Webbook
rinpol	576.00		NIST Webbook
rinpol	565.00		NIST Webbook
rinpol	567.00		NIST Webbook
rinpol	564.00		NIST Webbook
rinpol	563.00		NIST Webbook
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rinpol	565.00		NIST Webbook
rinpol	565.00		NIST Webbook
rinpol	565.00		NIST Webbook
rinpol	563.00		NIST Webbook
rinpol	568.00		NIST Webbook
rinpol	578.00		NIST Webbook
rinpol	575.00		NIST Webbook
rinpol	575.00		NIST Webbook
rinpol	563.30		NIST Webbook
rinpol	564.00		NIST Webbook
rinpol	567.00		NIST Webbook
rinpol	560.70		NIST Webbook
rinpol	563.30		NIST Webbook
rinpol	562.80		NIST Webbook
rinpol	562.70		NIST Webbook
rinpol	562.80		NIST Webbook
rinpol	575.00		NIST Webbook
rinpol	575.00		NIST Webbook
rinpol	566.00		NIST Webbook
rinpol	581.60		NIST Webbook
tb	332.60	K	NIST Webbook
tb	332.61 ± 0.30	K	NIST Webbook

tb	332.70 ± 0.40	K	NIST Webbook
tb	332.30 ± 0.50	K	NIST Webbook
tb	332.55 ± 0.50	K	NIST Webbook
tb	332.60	K	KDB
tb	332.00 ± 4.00	K	NIST Webbook
tb	332.82 ± 1.00	K	NIST Webbook
tb	333.00 ± 3.00	K	NIST Webbook
tb	333.65 ± 1.50	K	NIST Webbook
tb	334.00 ± 2.00	K	NIST Webbook
tb	332.65 ± 0.20	K	NIST Webbook
tb	333.00	K	NIST Webbook
tb	332.67 ± 0.20	K	NIST Webbook
tb	332.40 ± 1.00	K	NIST Webbook
tc	508.00	K	NIST Webbook
tc	508.00	K	KDB
tf	132.50 ± 0.20	K	NIST Webbook
tf	132.40 ± 0.50	K	NIST Webbook
tf	132.00 ± 0.50	K	NIST Webbook
tf	132.40	K	KDB
tf	132.50 ± 0.20	K	NIST Webbook
tf	132.44 ± 0.04	K	NIST Webbook
tf	132.10 ± 0.50	K	NIST Webbook
tf	132.25	K	Aqueous Solubility Prediction Method
vc	0.334	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.19	J/mol×K	500.25	Joback Method
cpg	175.75	J/mol×K	471.88	Joback Method
cpg	167.96	J/mol×K	443.51	Joback Method
cpg	159.81	J/mol×K	415.14	Joback Method
cpg	151.29	J/mol×K	386.78	Joback Method
cpg	142.39	J/mol×K	358.41	Joback Method
cpg	133.09	J/mol×K	330.04	Joback Method
cpl	133.10	J/mol×K	298.00	NIST Webbook
dvisc	0.0002043	Pa×s	330.04	Joback Method
dvisc	0.0002547	Pa×s	300.68	Joback Method
dvisc	0.0012470	Pa×s	183.22	Joback Method
dvisc	0.0007111	Pa×s	212.59	Joback Method

dvisc	0.0004647	Pa×s	241.95	Joback Method
dvisc	0.0003330	Pa×s	271.31	Joback Method
dvisc	0.0027097	Pa×s	153.86	Joback Method
hvapt	29.40	kJ/mol	316.00	NIST Webbook
hvapt	30.50	kJ/mol	303.00	NIST Webbook
hvapt	28.60	kJ/mol	309.50	NIST Webbook
pvap	109.00	kPa	333.00	Vapor Liquid Equilibria of the Binary System 1,5-Hexadiene + Allyl Chloride
pvap	256.00	kPa	362.75	Vapor Liquid Equilibria of the Binary System 1,5-Hexadiene + Allyl Chloride
pvap	197.00	kPa	352.84	Vapor Liquid Equilibria of the Binary System 1,5-Hexadiene + Allyl Chloride
pvap	78.00	kPa	322.92	Vapor Liquid Equilibria of the Binary System 1,5-Hexadiene + Allyl Chloride
pvap	303.00	kPa	369.36	Vapor Liquid Equilibria of the Binary System 1,5-Hexadiene + Allyl Chloride
pvap	56.00	kPa	313.05	Vapor Liquid Equilibria of the Binary System 1,5-Hexadiene + Allyl Chloride
pvap	316.61	kPa	373.10	Vapor-Liquid Equilibria on Seven Binary Systems: Ethylene Oxide + 2-Methylpropane; Acetophenone + Phenol; cis-1,3-Dichloropropene + 1,2-Dichloropropane; 1,5-Hexadiene + Allyl Chloride; Isopropyl Acetate + Acetonitrile; Vinyl Chloride + Methyl Chloride; and 1,4-Butanediol + c-Butyrolactone

pvap	103.15	kPa	333.15	Vapor-Liquid Equilibria on Seven Binary Systems: Ethylene Oxide + 2-Methylpropane; Acetophenone + Phenol; cis-1,3-Dichloropropene + 1,2-Dichloropropane; 1,5-Hexadiene + Allyl Chloride; Isopropyl Acetate + Acetonitrile; Vinyl Chloride + Methyl Chloride; and 1,4-Butanediol + c-Butyrolactone
pvap	147.00	kPa	342.76	Vapor Liquid Equilibria of the Binary System 1,5-Hexadiene + Allyl Chloride
rfi	1.40100		298.15	KDB
rhol	692.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41863e+01
Coeff. B	-2.91748e+03
Coeff. C	-2.80800e+01
Temperature range (K), min.	237.99
Temperature range (K), max.	356.81

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.38501e+01
Coeff. B	-5.15837e+03
Coeff. C	-5.89548e+00
Coeff. D	4.41960e-06
Temperature range (K), min.	132.47
Temperature range (K), max.	507.00

Sources

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/mol371.mol
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Relation between characteristic molecular volume and hydrophobicity of nonpolar molecules:	https://www.doi.org/10.1016/j.jct.2010.04.011
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=371
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Vapor-Liquid Equilibria on Seven Binary Systems: Ethylene Oxide + 2-Methylpropane; Acetophenone + Phenol; cis-1,3-Dichloropropene + 1,2-Dichloropropane; 1,5-Hexadiene + Allyl Chloride; Isopropyl Acetate + Acetonitrile; Vinyl Chloride + Methyl Chloride and 1,4-Butanediol + c-Butyrolactone:	https://www.doi.org/10.1021/je050317k
Vapor-Liquid Equilibria of the Binary System 1,5-Hexadiene + Allyl Chloride:	https://www.doi.org/10.1021/je400755x
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C592427&Units=SI

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume