1-Butene

Other names:	1-Butylene
	1-C4H8
	BUT-1-ENE
	BUTENE-1
	ETHYLETHYLENE
	«alpha»-Butene
	«alpha»-Butylene
	Â«alphaÂ»-Butene
	Â«alphaÂ»-Butylene
Inchi:	InChI=1S/C4H8/c1-3-4-2/h3H,1,4H2,2H3
InchiKey:	VXNZUUAINFGPBY-UHFFFAOYSA-N
Formula:	C4H8
SMILES:	C=CCC
Mol. weight [g/mol]:	56.11
CAS:	106-98-9

Physical Properties

Property code	Value	Unit	Source
af	0.1910		KDB
aigt	658.15	K	KDB
chg	-2716.80 ± 0.75	kJ/mol	NIST Webbook
dm	0.30	debye	KDB
fll	1.60	% in Air	KDB
flu	10.00	% in Air	KDB
gf	71.34	kJ/mol	KDB
gyrad	2.7460		KDB
hcg	2696.55	kJ/mol	KDB
hcn	2520.483	kJ/mol	KDB
hf	-0.13	kJ/mol	KDB
hf	-0.63 ± 0.79	kJ/mol	NIST Webbook
hfus	4.84	kJ/mol	Joback Method
hvap	20.88	kJ/mol	NIST Webbook
hvap	20.10	kJ/mol	NIST Webbook
ie	9.58	eV	NIST Webbook
ie	9.58 ± 0.01	eV	NIST Webbook
ie	9.77 ± 0.01	eV	NIST Webbook
ie	9.61 ± 0.02	eV	NIST Webbook

ie	10.00	eV	NIST Webbook
ie	9.62 ± 0.00	eV	NIST Webbook
ie	9.62	eV	NIST Webbook
ie	9.72	eV	NIST Webbook
ie	9.55 ± 0.06	eV	NIST Webbook
ie	9.55 ± 0.06	eV	NIST Webbook
ie	9.57	eV	NIST Webbook
ie	9.59	eV	NIST Webbook
ie	9.62 ± 0.05	eV	NIST Webbook
ie	9.59 ± 0.02	eV	NIST Webbook
ie	9.63 ± 0.02	eV	NIST Webbook
ie	9.58	eV	NIST Webbook
log10ws	-1.94		Aqueous Solubility Prediction Method
log10ws	-1.94		Estimated Solubility Method
logp	1.582		Crippen Method
mcvol	62.920	ml/mol	McGowan Method
nfpaf	%!d(float64=4)		KDB
nfpah	%!d(float64=1)		KDB
pc	4005.10	kPa	Thermodynamic properties of the butenes Part I. Experimental densities, vapor pressures, and critical points
pc	4000.00	kPa	Critical Temperatures and Pressures of Several Binary and Ternary Mixtures Concerning the Alkylation of 2-Methylpropane with 1-Butene in the Presence of Methane or Carbon Dioxide
pc	4020.00	kPa	KDB
pc	4020.00 ± 50.00	kPa	NIST Webbook
rhoc	232.84 ± 2.81	kg/m3	NIST Webbook
rinpol	385.00		NIST Webbook
rinpol	394.00		NIST Webbook
rinpol	389.20		NIST Webbook
rinpol	388.70		NIST Webbook
rinpol	384.00		NIST Webbook
rinpol	394.00		NIST Webbook
rinpol	394.00		NIST Webbook
rinpol	391.00		NIST Webbook
rinpol	389.00		NIST Webbook
rinpol	390.00		NIST Webbook
rinpol	388.70		NIST Webbook
rinpol	391.00		NIST Webbook

rinpol	390.00	NIST Webbook
rinpol	386.00	NIST Webbook
rinpol	384.40	NIST Webbook
rinpol	384.00	NIST Webbook
rinpol	395.00	NIST Webbook
rinpol	385.00	NIST Webbook
rinpol	385.00	NIST Webbook
rinpol	385.00	NIST Webbook
rinpol	385.00	NIST Webbook
rinpol	385.00	NIST Webbook
rinpol	393.00	NIST Webbook
rinpol	385.00	NIST Webbook
rinpol	389.20	NIST Webbook
rinpol	392.00	NIST Webbook
rinpol	386.00	NIST Webbook
rinpol	400.00	NIST Webbook
rinpol	388.00	NIST Webbook
rinpol	385.00	NIST Webbook
rinpol	402.00	NIST Webbook
rinpol	400.00	NIST Webbook
rinpol	390.00	NIST Webbook
rinpol	392.00	NIST Webbook
rinpol	382.00	NIST Webbook
rinpol	385.00	NIST Webbook
rinpol	385.00	NIST Webbook
rinpol	385.00	NIST Webbook
rinpol	388.00	NIST Webbook
rinpol	386.00	NIST Webbook
rinpol	387.00	NIST Webbook
rinpol	386.00	NIST Webbook
rinpol	390.00	NIST Webbook
rinpol	384.00	NIST Webbook
rinpol	391.00	NIST Webbook
rinpol	383.00	NIST Webbook
rinpol	387.00	NIST Webbook
rinpol	386.00	NIST Webbook
rinpol	392.00	NIST Webbook
rinpol	387.00	NIST Webbook
rinpol	387.00	NIST Webbook
rinpol	387.00	NIST Webbook
rinpol	386.00	NIST Webbook
rinpol	390.00	NIST Webbook
rinpol	390.00	NIST Webbook
rinpol	386.00	NIST Webbook

ripol	415.00		NIST Webbook
ripol	436.00		NIST Webbook
ripol	415.00		NIST Webbook
ripol	436.00		NIST Webbook
ripol	426.00		NIST Webbook
sl	227.00	J/mol×K	NIST Webbook
sl	229.06	J/mol×K	NIST Webbook
sl	213.84	J/mol×K	NIST Webbook
tb	266.89	K	KDB
tc	419.50 ± 0.50	K	NIST Webbook
tc	417.15 ± 2.00	K	NIST Webbook
tc	419.60	K	NIST Webbook
tc	419.50	K	KDB
tf	87.80	K	KDB
tf	87.93	K	Aqueous Solubility Prediction Method
tt	87.80 ± 0.05	K	NIST Webbook
tt	87.80 ± 0.01	K	NIST Webbook
tt	87.83 ± 0.05	K	NIST Webbook
tt	87.82 ± 0.02	K	NIST Webbook
vc	0.241	m3/kmol	KDB
vc	0.241	m3/kmol	NIST Webbook
zc	0.2775330		KDB
zra	0.27		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	89.58 ± 0.06	J/mol×K	313.55	NIST Webbook
cpg	101.21 ± 0.07	J/mol×K	363.25	NIST Webbook
cpl	128.96	J/mol×K	298.15	NIST Webbook
cpl	118.00	J/mol×K	298.15	NIST Webbook
cpl	128.60	J/mol×K	294.00	NIST Webbook
cpl	119.45	J/mol×K	260.00	NIST Webbook
cpl	119.16	J/mol×K	253.40	NIST Webbook
dvisc	0.0020285	Pa×s	133.08	Joback Method
dvisc	0.0005506	Pa×s	184.59	Joback Method
dvisc	0.0001647	Pa×s	287.60	Joback Method
dvisc	0.0002038	Pa×s	261.85	Joback Method
dvisc	0.0002640	Pa×s	236.09	Joback Method
dvisc	0.0003645	Pa×s	210.34	Joback Method

dvisc	0.0009508	Pa×s	158.83	Joback Method
hfust	3.85	kJ/mol	87.80	NIST Webbook
hfust	3.96	kJ/mol	87.81	NIST Webbook
hfust	3.85	kJ/mol	87.82	NIST Webbook
hfust	3.85	kJ/mol	87.82	NIST Webbook
hfust	3.85	kJ/mol	87.80	NIST Webbook
hvapt	25.30	kJ/mol	202.00	NIST Webbook
hvapt	23.20	kJ/mol	244.50	NIST Webbook
hvapt	23.30	kJ/mol	242.00	NIST Webbook
hvapt	24.50	kJ/mol	219.00	NIST Webbook
hvapt	23.70	kJ/mol	202.00	NIST Webbook
hvapt	22.50	kJ/mol	339.00	NIST Webbook
hvapt	22.00	kJ/mol	376.50	NIST Webbook
hvapt	28.30	kJ/mol	159.00	NIST Webbook
hvapt	23.30	kJ/mol	237.00	NIST Webbook
hvapt	22.07	kJ/mol	266.90	NIST Webbook
hvapt	21.92	kJ/mol	266.90	KDB
hvapt	21.87	kJ/mol	266.91	NIST Webbook
hvapt	21.90	kJ/mol	267.00	NIST Webbook
hvapt	22.80	kJ/mol	306.00	NIST Webbook
pvap	596.14	kPa	323.27	Vapor-Liquid Equilibrium for 1-Propanol + 1-Butene, + cis-2-Butene, + 2-Methyl-propene, + trans-2-Butene, + n-Butane, and + 2-Methyl-propane
pvap	1510.50	kPa	364.51	Vapor Liquid Equilibrium for Six Binary Systems of C4-Hydrocarbons + 2-Propanone
pvap	525.20	kPa	318.32	Vapor-Liquid Equilibrium for 1-Butanol + 1-Butene at (318.4 and 364.5) K and Vapor-Liquid Equilibrium of 1-Butanol + 2-Methylpropane, + n-Butane and 1-Butene + 2-Methylpropane at 318.4 K

pvap	1197.00	kPa	353.18	Experimental vapour liquid equilibrium data and modeling for binary mixtures of 1-butene with 1,1,2,3,3,3-hexafluoro-1-propene, 2,2,3-trifluoro-3-(trifluoromethyl)oxirane, or difluoromethane
pvap	525.80	kPa	318.40	Vapor-Liquid Equilibrium for 1-Butanol + 1-Butene at (318.4 and 364.5) K and Vapor-Liquid Equilibrium of 1-Butanol + 2-Methylpropane, + n-Butane and 1-Butene + 2-Methylpropane at 318.4 K
pvap	855.00	kPa	337.99	Experimental vapour liquid equilibrium data and modeling for binary mixtures of 1-butene with 1,1,2,3,3,3-hexafluoro-1-propene, 2,2,3-trifluoro-3-(trifluoromethyl)oxirane, or difluoromethane
pvap	525.55	kPa	318.42	Vapour liquid equilibrium for the ethyl ethanoate + 1-butene, +cis-2-butene, +trans-2-butene, +2-methylpropene, +n-butane and +2-methylpropane
pvap	454.50	kPa	312.57	Isothermal binary vapour liquid equilibrium for butanes and butenes with dimethylsulphide
pvap	451.30	kPa	312.58	Vapour liquid equilibrium for the systems diethyl sulphide + 1-butene, +cis-2-butene, +2-methylpropane, +2-methylpropene, +n-butane, +trans-2-butene

pvap	448.30	kPa	312.59	Phase equilibrium measurements for systems containing propanenitrile with tert-butyl ethyl ether and C4-hydrocarbons
pvap	343.00	kPa	302.90	Experimental vapour liquid equilibrium data and modeling for binary mixtures of 1-butene with 1,1,2,3,3,3-hexafluoro-1-propene, 2,2,3-trifluoro-3-(trifluoromethyl)oxirane, or difluoromethane
pvap	957.00	kPa	342.98	Experimental vapour liquid equilibrium data and modeling for binary mixtures of 1-butene with 1,1,2,3,3,3-hexafluoro-1-propene, 2,2,3-trifluoro-3-(trifluoromethyl)oxirane, or difluoromethane
pvap	456.00	kPa	312.96	Experimental vapour liquid equilibrium data and modeling for binary mixtures of 1-butene with 1,1,2,3,3,3-hexafluoro-1-propene, 2,2,3-trifluoro-3-(trifluoromethyl)oxirane, or difluoromethane
pvap	521.00	kPa	318.05	Experimental vapour liquid equilibrium data and modeling for binary mixtures of 1-butene with 1,1,2,3,3,3-hexafluoro-1-propene, 2,2,3-trifluoro-3-(trifluoromethyl)oxirane, or difluoromethane
pvap	593.00	kPa	322.94	Experimental vapour liquid equilibrium data and modeling for binary mixtures of 1-butene with 1,1,2,3,3,3-hexafluoro-1-propene, 2,2,3-trifluoro-3-(trifluoromethyl)oxirane, or difluoromethane

pvap	671.00	kPa	328.06	Experimental vapour liquid equilibrium data and modeling for binary mixtures of 1-butene with 1,1,2,3,3,3-hexafluoro-1-propene, 2,2,3-trifluoro-3-(trifluoromethyl)oxirane, or difluoromethane
pvap	759.00	kPa	332.97	Experimental vapour liquid equilibrium data and modeling for binary mixtures of 1-butene with 1,1,2,3,3,3-hexafluoro-1-propene, 2,2,3-trifluoro-3-(trifluoromethyl)oxirane, or difluoromethane
pvap	396.00	kPa	307.83	Experimental vapour liquid equilibrium data and modeling for binary mixtures of 1-butene with 1,1,2,3,3,3-hexafluoro-1-propene, 2,2,3-trifluoro-3-(trifluoromethyl)oxirane, or difluoromethane
pvap	1509.40	kPa	364.53	Vapor-Liquid Equilibrium for 1-Butanol + 1-Butene at (318.4 and 364.5) K and Vapor-Liquid Equilibrium of 1-Butanol + 2-Methylpropane, + n-Butane and 1-Butene + 2-Methylpropane at 318.4 K
pvap	1069.00	kPa	347.93	Experimental vapour liquid equilibrium data and modeling for binary mixtures of 1-butene with 1,1,2,3,3,3-hexafluoro-1-propene, 2,2,3-trifluoro-3-(trifluoromethyl)oxirane, or difluoromethane
rhol	595.00	kg/m3	293.00	KDB
sfust	43.80	J/mol×K	87.82	NIST Webbook
sfust	43.83	J/mol×K	87.82	NIST Webbook
sfust	45.09	J/mol×K	87.81	NIST Webbook

srf	0.01	N/m	293.20	KDB
svapt	81.92	J/mol×K	266.91	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41892e+01
Coeff. B	-2.33475e+03
Coeff. C	-2.28580e+01
Temperature range (K), min.	190.81
Temperature range (K), max.	285.85

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.43474e+01
Coeff. B	-4.50983e+03
Coeff. C	-7.78979e+00
Coeff. D	9.81623e-06
Temperature range (K), min.	87.80
Temperature range (K), max.	419.59

Sources

Influence of a-Olefin Concentration and Length on the High-Pressure Phase Behavior of (a-Olefin + n-Hexane + LDPE) Systems:	https://www.doi.org/10.1021/acs.jced.9b00224
Henry's constants and infinite dilution activity coefficients of propane, propene, butane, isobutane, 1-butene, isobutene, trans-2-butene, and 1,3-butadiene in isobutanol and tert-butanol:	https://www.doi.org/10.1016/j.jct.2004.05.010
Henry's law constants and infinite dilution activity coefficients of propane, propene, butane, isobutane, 1-butene, isobutene, trans-2-butene, and 1,3-butadiene in 2-methyl-1-butanol, 3-methyl-1-butanol, and 2-methyl-2-butanol:	https://www.doi.org/10.1021/je049723e
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Henry's constants and infinite dilution activity coefficients of propane, propene, butane, isobutane, 1-butene, isobutene, trans-2-butene, and 1,3-butadiene in 1-pentanol, 2-pentanol and 3-pentanol:	https://www.doi.org/10.1016/j.jct.2004.11.005
Solubilities of Gases in the Ionic Liquid 1-n-Butyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide:	https://www.doi.org/10.1021/je050357o
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Henry's law constants of 1-butene, 2-methylpropene, trans-2-butene, and 1,3-butadiene in methanol at 374 490K:	https://www.doi.org/10.1016/j.fluid.2006.06.024
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106989&Units=SI
Vapor-Liquid Equilibrium for 1-Butene + Methanol, + 1-Propanol, + 2-Propanol, + 2-Butanol, and 2-Methyl-2-propanol (TBA) at 364.5 K:	https://www.doi.org/10.1021/je800160q
Isothermal binary vapour-liquid equilibrium for butanes and butenes with dimethylsulphide:	https://www.doi.org/10.1016/j.fluid.2008.01.030

Vapor Liquid Equilibrium for Six Binary Systems of C4-Hydrocarbons + 2-Propanone:	https://www.doi.org/10.1021/je050403k
Henry's Law Constants and Infinite Dilution Activity Coefficients of Propane, Propene, Butane, 2-Methylpropane, 1-Butene, 2-Methylpropene, trans-2-Butene, cis-2-Butene, 1,3-Butadiene, Dimethyl Ether, Chloroethane, and 1,1-Difluoroethane in 2-Propen-1-ol:	https://www.doi.org/10.1021/je050343i
Henry's Law Constants and Infinite Dilution Activity Coefficients of Propane, Propene, Butane, 2-Methylpropane, 1-Butene, 2-Methylpropene, trans-2-Butene, cis-2-Butene, 1,3-Butadiene, Dimethyl Ether, Chloroethane, and 1,1-Difluoroethane in 2-Methyl-3-buten-2-ol and 3-Methyl-2-buten-1-ol:	https://www.doi.org/10.1021/je0502647
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB:	https://www.cheric.org/files/research/kdb/mol/mol186.mol
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=186
Henry's Constants and Infinite Dilution Activity Coefficients of Propane, Propene, Butane, Isobutane, 1-Butene, Isobutene, trans-2-Butene and 1,3-Butadiene in 1-Butanol and 2-Butanol at (250 to 330) K:	https://www.doi.org/10.1021/je034265f
Henry's Law Constants and Infinite Dilution Activity Coefficients of Propane, Propene, Butane, 2-Methylpropane, 1-Butene, 2-Methylpropene, trans-2-Butene, cis-2-Butene, 1,3-Butadiene, Dimethylether, Chloroethane, 1,1-Difluoroethane, and Hexane in Tetrahydropyran:	https://www.doi.org/10.1021/je700270d
Vapour liquid equilibrium for the ethyl ethanoate + 1-butene, cis-2-butene, 2-methylpropene:	https://www.doi.org/10.1016/j.fluid.2004.10.023
Henry's Constants and Infinite Dilution Activity Coefficients of Propane, Propene, Butane, Isobutane, 1-Butene, Isobutene, trans-2-Butene and 1,3-Butadiene in 2-Propanol at 250-330 K:	https://www.doi.org/10.1021/je0342116
Thermodynamic properties of the butenes. Part II. Experimental densities, vapour pressures and critical points:	https://www.doi.org/10.1016/j.fluid.2004.09.013
Experimental vapour liquid equilibrium data and modelling for binary mixtures of decafluorobutane with propane and 1-butene:	https://www.doi.org/10.1016/j.jct.2013.07.020
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Phase equilibrium measurements for systems containing propanenitrile with tert-butylmethyl ether and C4-hydrocarbons:	https://www.doi.org/10.1016/j.fluid.2010.09.023
Vapor-Liquid Equilibrium for 1-Butanol + 1-Butene at (318.4 and 364.5) K and Vapor-Liquid Equilibrium of 1-Butanol + 2-Methylpropane, + n-Butane and 1-Butene + 2-Methylpropane at 318.4 K:	https://www.doi.org/10.1021/je8004672
Vapour liquid equilibrium for the systems diethyl sulphide + 1-butene, + cis-2-butene, +2-methylpropene, +n-butane, +trans-2-butene:	https://www.doi.org/10.1016/j.fluid.2010.01.006
Henry's constants and infinite dilution activity coefficients of propane, propene, butane, isobutane, 1-butene, isobutene, trans-2-butene and 1,3-butadiene in 1-propanol at T=(260 to 340) K:	https://www.doi.org/10.1016/j.jct.2003.08.018
Experimental vapour-liquid equilibrium data and modeling for binary mixtures of 1-butene with 1,1,2,3,3,3-hexafluoro-1-propene, 2,2,3-trifluoro-3-(trifluoromethyl)oxirane, or difluoromethane:	https://www.doi.org/10.1016/j.jct.2013.01.017
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Henry's Law Constants and Infinite Dilution Activity Coefficients of Propane, Propene, Butane, 2-Methylpropane, 1-Butene, 2-Methylpropene, trans-2-Butene, cis-2-Butene, 1,3-Butadiene, Dimethyl Ether, Chloroethane, and 1,1-Difluoroethane in Benzene, Toluene, o-Xylene, m-Xylene, p-Xylene, and Styrene:	https://www.doi.org/10.1021/je060395n
Critical Temperatures and Pressures of Several Binary and Ternary Mixtures Concerning the Alkylation of 2-Methylpropane with 1-Butene in the Presence of Methane or Carbon Dioxide:	https://www.doi.org/10.1021/je700132w
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=186
Vapor-Liquid Equilibrium for 1-Propanol + 1-Butene, + cis-2-Butene, + 2-Methyl-propene, + trans-2-Butene, + n-Butane, and + 2-Methyl-propane:	https://www.doi.org/10.1021/je049959i
Henry's Law Constants and Infinite Dilution Activity Coefficients of Propane, Propene, Butane, 2-Methylpropane, 1-Butene, 2-Methylpropene, trans-2-Butene, cis-2-Butene, 1,3-Butadiene, Dimethyl Ether, Chloroethane, and 1,1-Difluoroethane in 2-Methylphenol, 3-Methylphenol, and 4-Methylphenol:	https://www.doi.org/10.1021/je100529s

Legend

af:	Acentric Factor
aigt:	Autoignition Temperature
chg:	Standard gas enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
fll:	Lower Flammability Limit
flu:	Upper Flammability Limit
gf:	Standard Gibbs free energy of formation
gyrad:	Radius of Gyration
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
svapt:	Entropy of vaporization at a given temperature
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