

# 1,3-Butadiene

<b>Other names:</b>	.alpha.,.gamma.-butadiene BIETHYLENE BIVINYL Buta-1,3-dieen Buta-1,3-dien Buta-1,3-diene Butadiéen Butadien Butadiene CH <sub>2</sub> =CHCH=CH <sub>2</sub> Divinyl Erythrene NCI-C50602 Pyrrolylene TRANS-BUTADIENE Vinylethylene butadiene-1,3 «alpha», «gamma»-Butadiene Â«alphaÂ»,Â«gammaÂ»-Butadiene
<b>Inchi:</b>	InChI=1S/C4H6/c1-3-4-2/h3-4H,1-2H2
<b>InchiKey:</b>	KAKZBPTYRLMSJV-UHFFFAOYSA-N
<b>Formula:</b>	C <sub>4</sub> H <sub>6</sub>
<b>SMILES:</b>	C=CC=C
<b>Mol. weight [g/mol]:</b>	54.09
<b>CAS:</b>	106-99-0

## Physical Properties

Property code	Value	Unit	Source
af	0.1950		KDB
affp	783.40	kJ/mol	NIST Webbook
aigt	693.15	K	KDB
basg	757.60	kJ/mol	NIST Webbook
chg	-2540.40 ± 0.75	kJ/mol	NIST Webbook
chl	-2522.10 ± 0.96	kJ/mol	NIST Webbook
dm	0.00	debye	KDB
fl	2.00	% in Air	KDB
flu	11.50	% in Air	KDB

fpc	197.04	K	KDB
fpo	197.04	K	KDB
gf	150.80	kJ/mol	KDB
hcg	2520.11	kJ/mol	KDB
hcn	2388.060	kJ/mol	KDB
hf	108.80 ± 0.79	kJ/mol	NIST Webbook
hf	111.90 ± 0.96	kJ/mol	NIST Webbook
hf	110.20	kJ/mol	KDB
hfl	90.50 ± 0.96	kJ/mol	NIST Webbook
hfus	3.56	kJ/mol	Joback Method
hvap	21.10	kJ/mol	NIST Webbook
hvap	21.47	kJ/mol	NIST Webbook
ie	9.06	eV	NIST Webbook
ie	9.03	eV	NIST Webbook
ie	9.07	eV	NIST Webbook
ie	9.06 ± 0.01	eV	NIST Webbook
ie	9.07	eV	NIST Webbook
ie	9.09	eV	NIST Webbook
ie	9.07 ± 0.01	eV	NIST Webbook
ie	9.09 ± 0.03	eV	NIST Webbook
ie	9.03 ± 0.02	eV	NIST Webbook
ie	9.08 ± 0.00	eV	NIST Webbook
ie	9.18 ± 0.04	eV	NIST Webbook
ie	9.07 ± 0.01	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.03	eV	NIST Webbook
ie	9.07	eV	NIST Webbook
ie	9.07 ± 0.02	eV	NIST Webbook
ie	9.09 ± 0.05	eV	NIST Webbook
ie	9.06 ± 0.02	eV	NIST Webbook
ie	9.03	eV	NIST Webbook
ie	9.07 ± 0.01	eV	NIST Webbook
log10ws	-1.87		Estimated Solubility Method
log10ws	-1.87		Aqueous Solubility Prediction Method
logp	1.358		Crippen Method
mcvol	58.620	ml/mol	McGowan Method
nfpaf	%!d(float64=4)		KDB
nfpah	%!d(float64=2)		KDB
nfpas	%!d(float64=2)		KDB
pc	4320.00	kPa	KDB
pc	4320.00 ± 100.00	kPa	NIST Webbook
rhoc	245.03 ± 5.41	kg/m3	NIST Webbook
rinpol	392.00		NIST Webbook

rinpol	396.00		NIST Webbook
rinpol	395.00		NIST Webbook
rinpol	386.00		NIST Webbook
rinpol	400.00		NIST Webbook
rinpol	390.00		NIST Webbook
rinpol	395.00		NIST Webbook
rinpol	398.00		NIST Webbook
rinpol	389.00		NIST Webbook
rinpol	395.00		NIST Webbook
rinpol	394.00		NIST Webbook
rinpol	390.00		NIST Webbook
rinpol	404.00		NIST Webbook
rinpol	393.00		NIST Webbook
rinpol	400.00		NIST Webbook
rinpol	400.00		NIST Webbook
rinpol	394.30		NIST Webbook
rinpol	397.00		NIST Webbook
rinpol	385.60		NIST Webbook
rinpol	386.00		NIST Webbook
rinpol	386.00		NIST Webbook
rinpol	387.00		NIST Webbook
rinpol	388.00		NIST Webbook
rinpol	405.00		NIST Webbook
rinpol	389.00		NIST Webbook
rinpol	393.00		NIST Webbook
rinpol	395.00		NIST Webbook
rinpol	403.00		NIST Webbook
rinpol	395.00		NIST Webbook
rinpol	395.00		NIST Webbook
rinpol	389.00		NIST Webbook
rinpol	412.00		NIST Webbook
ripol	487.00		NIST Webbook
ripol	507.00		NIST Webbook
sl	199.00	J/molxK	NIST Webbook
tb	268.74	K	KDB
tc	425.00 ± 1.00	K	NIST Webbook
tc	425.00	K	KDB
tc	425.00	K	NIST Webbook
tf	162.20	K	Aqueous Solubility Prediction Method
tf	164.20	K	KDB
tt	164.24 ± 0.02	K	NIST Webbook
vc	0.221	m3/kmol	NIST Webbook
vc	0.221	m3/kmol	KDB
zc	0.2701780		KDB

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	73.28	J/molxK	284.28	Joback Method
cpg	79.44	J/molxK	312.30	Joback Method
cpg	106.36	J/molxK	452.41	Joback Method
cpg	101.46	J/molxK	424.39	Joback Method
cpg	96.33	J/molxK	396.37	Joback Method
cpg	90.96	J/molxK	368.35	Joback Method
cpg	85.33	J/molxK	340.32	Joback Method
cpl	123.65	J/molxK	298.15	NIST Webbook
dvisc	0.0003054	Paxs	207.80	Joback Method
dvisc	0.0001485	Paxs	284.28	Joback Method
dvisc	0.0001801	Paxs	258.79	Joback Method
dvisc	0.0002279	Paxs	233.29	Joback Method
dvisc	0.0007297	Paxs	156.81	Joback Method
dvisc	0.0014538	Paxs	131.32	Joback Method
dvisc	0.0004442	Paxs	182.31	Joback Method
hfust	7.98	kJ/mol	164.20	NIST Webbook
hfust	7.98	kJ/mol	164.24	NIST Webbook
hfust	7.98	kJ/mol	164.20	NIST Webbook
hvapt	24.70	kJ/mol	220.00	NIST Webbook
hvapt	23.70	kJ/mol	234.50	NIST Webbook
hvapt	22.90	kJ/mol	402.50	NIST Webbook
hvapt	22.40	kJ/mol	348.50	NIST Webbook
hvapt	25.70	kJ/mol	203.00	NIST Webbook
hvapt	23.00	kJ/mol	294.00	NIST Webbook
hvapt	0.08	kJ/mol	273.15	NIST Webbook
hvapt	22.47	kJ/mol	268.70	NIST Webbook
hvapt	22.47	kJ/mol	268.70	KDB
hvapt	23.60	kJ/mol	244.50	NIST Webbook
rho1	621.00	kg/m3	293.00	KDB
sfust	48.61	J/molxK	164.24	NIST Webbook
srf	0.02	N/m	233.20	KDB
svapt	280.64	J/molxK	273.15	NIST Webbook



# Legend

<b>af:</b>	Acentric Factor
<b>affp:</b>	Proton affinity
<b>aigt:</b>	Autoignition Temperature
<b>basg:</b>	Gas basicity
<b>chg:</b>	Standard gas enthalpy of combustion
<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>cpl:</b>	Liquid phase heat capacity
<b>dm:</b>	Dipole Moment
<b>dvisc:</b>	Dynamic viscosity
<b>fl:</b>	Lower Flammability Limit
<b>flu:</b>	Upper Flammability Limit
<b>fpc:</b>	Flash Point (Closed Cup Method)
<b>fpo:</b>	Flash Point (Open Cup Method)
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hcg:</b>	Heat of Combustion, Gross form
<b>hcn:</b>	Heat of Combustion, Net Form
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfl:</b>	Liquid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>nfpaf:</b>	NFPA Fire Rating
<b>nfpah:</b>	NFPA Health Rating
<b>nfpas:</b>	NFPA Safety Rating
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rhoc:</b>	Critical density
<b>rho:</b>	Liquid Density
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>sfust:</b>	Entropy of fusion at a given temperature
<b>sl:</b>	Liquid phase molar entropy at standard conditions
<b>srf:</b>	Surface Tension

<b>svapt:</b>	Entropy of vaporization at a given temperature
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>tt:</b>	Triple Point Temperature
<b>vc:</b>	Critical Volume
<b>zc:</b>	Critical Compressibility
<b>zra:</b>	Rackett Parameter

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