1,2-Butadiene

Other names:	Allene, methyl- Buta-1,2-diene CH2=C=CHCH3 METHYLALLENE
Inchi:	InChI=1S/C4H6/c1-3-4-2/h4H,1H2,2H3
InchiKey:	QNRMTGGDHLBXQZ-UHFFFAOYSA-N
Formula:	C4H6
SMILES:	C=C=CC
Mol. weight [g/mol]:	54.09
CAS:	590-19-2

Physical Properties

Property code	Value	Unit	Source
af	0.2550		KDB
affp	778.90	kJ/mol	NIST Webbook
basg	749.80	kJ/mol	NIST Webbook
chg	-2597.00 ± 1.20	kJ/mol	NIST Webbook
chg	-2593.80 ± 0.54	kJ/mol	NIST Webbook
dm	0.40	debye	KDB
gf	198.60	kJ/mol	KDB
hcg	2569.52	kJ/mol	KDB
hcn	2437.515	kJ/mol	KDB
hf	162.20 ± 0.59	kJ/mol	NIST Webbook
hf	165.40 ± 1.20	kJ/mol	NIST Webbook
hf	162.30	kJ/mol	KDB
hfus	6.97	kJ/mol	Joback Method
hvap	23.90	kJ/mol	NIST Webbook
hvap	23.68	kJ/mol	NIST Webbook
ie	9.23 ± 0.02	eV	NIST Webbook
ie	9.33 ± 0.02	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
ie	9.03	eV	NIST Webbook
ie	9.33	eV	NIST Webbook
log10ws	-1.22		Crippen Method
logp	1.347		Crippen Method
mcvol	58.620	ml/mol	McGowan Method
pc	4490.00	kPa	KDB

rinpol	450.00		NIST Webbook
rinpol	428.50		NIST Webbook
rinpol	428.50		NIST Webbook
rinpol	427.90		NIST Webbook
rinpol	430.00		NIST Webbook
rinpol	430.00		NIST Webbook
rinpol	430.00		NIST Webbook
rinpol	430.00		NIST Webbook
rinpol	448.00		NIST Webbook
rinpol	427.00		NIST Webbook
rinpol	450.00		NIST Webbook
rinpol	441.00		NIST Webbook
rinpol	427.00		NIST Webbook
rinpol	429.00		NIST Webbook
ripol	562.00		NIST Webbook
ripol	540.00		NIST Webbook
ripol	562.00		NIST Webbook
sl	206.19	J/mol×K	NIST Webbook
tb	291.70 ± 2.00	K	NIST Webbook
tb	284.06 ± 0.30	K	NIST Webbook
tb	283.50 ± 0.50	K	NIST Webbook
tb	284.00	K	KDB
tb	284.00	K	NIST Webbook
tc	443.70	K	KDB
tf	136.94 ± 0.05	K	NIST Webbook
tf	137.00	K	KDB
tf	136.96 ± 0.02	K	NIST Webbook
tt	136.95 ± 0.05	K	NIST Webbook
tt	136.92 ± 0.06	K	NIST Webbook
tt	136.94 ± 0.08	K	NIST Webbook
vc	0.219	m3/kmol	KDB
zc	0.2665410		KDB
zra	0.27		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	96.14	J/mol×K	379.33	Joback Method
cpg	91.27	J/mol×K	349.84	Joback Method
cpg	86.28	J/mol×K	320.36	Joback Method
cpg	110.00	J/mol×K	467.79	Joback Method

cpg	105.51	J/mol×K	438.30	Joback Method
cpg	100.88	J/mol×K	408.82	Joback Method
cpg	81.17	J/mol×K	290.87	Joback Method
cpl	122.80	J/mol×K	290.00	NIST Webbook
hfust	6.95	kJ/mol	136.90	NIST Webbook
hfust	6.96	kJ/mol	136.90	NIST Webbook
hfust	6.96	kJ/mol	136.92	NIST Webbook
hvapt	25.20	kJ/mol	237.50	NIST Webbook
hvapt	25.30	kJ/mol	267.00	NIST Webbook
hvapt	24.02	kJ/mol	284.00	NIST Webbook
hvapt	24.62	kJ/mol	273.24	NIST Webbook
hvapt	24.60 ± 0.10	kJ/mol	273.00	NIST Webbook
hvapt	24.60 ± 0.30	kJ/mol	273.25	NIST Webbook
hvapt	26.40	kJ/mol	223.50	NIST Webbook
hvapt	24.27	kJ/mol	284.00	KDB
rhol	652.00	kg/m3	293.00	KDB
sfust	50.84	J/mol×K	136.92	NIST Webbook
srf	0.02	N/m	298.20	KDB
svapt	90.11	J/mol×K	273.24	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42524e+01
Coeff. B	-2.52653e+03
Coeff. C	-2.17500e+01
Temperature range (K), min.	202.67
Temperature range (K), max.	304.33

Sources

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/mol357.mol

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C590192&Units=SI

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chg:	Standard gas enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
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
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