1,2-Butadiene, 3-methyl-

Other names:	1,1-DIMETHYLALLENE
	1,1-DIMETHYLALLYLENE
	2-METHYL-2,3-BUTADIENE
	3,3-Dimethylallene
	3-Methyl-1,2-butadiene
	3-methylbuta-1,2-diene
	CH2=C=C(CH3)2
Inchi:	InChI=1S/C5H8/c1-4-5(2)3/h1H2,2-3H3
InchiKey:	PAKGDPSCXSUALC-UHFFFAOYSA-N
Formula:	C5H8
SMILES:	C=C=C(C)C
Mol. weight [g/mol]:	68.12
CAS:	598-25-4

Physical Properties

Property code	Value	Unit	Source
af	0.1600		KDB
chl	-3212.10 ± 0.42	kJ/mol	NIST Webbook
gf	198.70	kJ/mol	KDB
hcg	3212.06	kJ/mol	KDB
hcn	3035.994	kJ/mol	KDB
hf	129.10	kJ/mol	NIST Webbook
hf	129.07 ± 0.57	kJ/mol	NIST Webbook
hf	129.80	kJ/mol	KDB
hfl	101.20 ± 0.50	kJ/mol	NIST Webbook
hfus	8.25	kJ/mol	Joback Method
hvap	28.00	kJ/mol	NIST Webbook
hvap	27.90 ± 0.28	kJ/mol	NIST Webbook
ie	8.95 ± 0.02	eV	NIST Webbook
ie	8.90	eV	NIST Webbook
ie	8.95	eV	NIST Webbook
log10ws	-1.64		Crippen Method
logp	1.737		Crippen Method
mcvol	72.710	ml/mol	McGowan Method
pc	4110.00	kPa	KDB
rinpol	510.00		NIST Webbook
rinpol	526.00		NIST Webbook

rinpol	531.00		NIST Webbook
rinpol	524.00		NIST Webbook
rinpol	535.50		NIST Webbook
rinpol	513.00		NIST Webbook
rinpol	512.00		NIST Webbook
rinpol	532.00		NIST Webbook
rinpol	510.00		NIST Webbook
rinpol	531.00		NIST Webbook
rinpol	512.00		NIST Webbook
rinpol	511.00		NIST Webbook
rinpol	511.00		NIST Webbook
rinpol	510.00		NIST Webbook
ripol	634.00		NIST Webbook
ripol	612.00		NIST Webbook
sg	321.21	J/mol×K	NIST Webbook
sl	231.79	J/mol×K	NIST Webbook
tb	314.00	K	KDB
tc	496.00	K	KDB
tf	159.50	K	KDB
tf	159.51 ± 0.03	K	NIST Webbook
tf	159.51 ± 0.02	K	NIST Webbook
tf	159.52 ± 0.01	K	NIST Webbook
tt	159.53 ± 0.05	K	NIST Webbook
vc	0.267	m3/kmol	KDB
zc	0.2660940		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	142.27	J/mol×K	465.15	Joback Method
cpg	109.14	J/mol×K	313.63	Joback Method
cpg	116.18	J/mol×K	343.93	Joback Method
cpg	123.01	J/mol×K	374.24	Joback Method
cpg	129.63	J/mol×K	404.54	Joback Method
cpg	136.05	J/mol×K	434.84	Joback Method
cpg	148.28	J/mol×K	495.45	Joback Method
cpl	152.42	J/mol×K	298.15	NIST Webbook
cpl	151.10	J/mol×K	298.15	NIST Webbook
hfust	7.95	kJ/mol	159.50	NIST Webbook
hfust	7.96	kJ/mol	159.53	NIST Webbook
hfust	7.95	kJ/mol	159.50	NIST Webbook

hvapt	29.00	kJ/mol	296.50	NIST Webbook
hvapt	27.24	kJ/mol	314.00	KDB
hvapt	31.00	kJ/mol	240.00	NIST Webbook
hvapt	29.90	kJ/mol	287.50	NIST Webbook
hvapt	31.60	kJ/mol	227.50	NIST Webbook
rfi	1.41692		298.15	KDB
rhol	686.00	kg/m3	293.00	KDB
sfust	49.87	J/mol×K	159.53	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	1.41686e+01
Coeff. B	-2.61851e+03
Coeff. C	-3.78190e+01
Temperature range (K), min.	226.46
Temperature range (K), max.	333.46

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.02254e+01
Coeff. B	-5.23197e+03
Coeff. C	-6.85750e+00
Coeff. D	4.86827e-06
Temperature range (K), min.	159.53
Temperature range (K), max.	496.00

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol364.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C598254&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=364
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

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
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
hfl:	Liquid phase 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