1-Butene, 3-methyl-

Other names:	(CH3)2CHCH=CH2
	.alpha.-isoamylene
	2-Methyl-3-butene
	3,3-dimethylpropene
	3-Methyl-1-butene
	3-Methylbutene-1
	3-methylbut-1-ene
	ISOPENTENE
	ISOPROPYLETHYLENE
	UN 2371
	UN 2561
	VINYLISOPROPYL
	isopropylethene
	«alpha»-Isoamylene
	Â«alphaÂ»-Isoamylene
Inchi:	InChI=1S/C5H10/c1-4-5(2)3/h4-5H,1H2,2-3H3
InchiKey:	YHQXBTXEYZIYOV-UHFFFAOYSA-N
Formula:	C5H10
SMILES:	C=CC(C)C
Mol. weight [g/mol]:	70.13
CAS:	563-45-1

Physical Properties

Property code	Value	Unit	Source
af	0.2090		KDB
chl	-3345.10 ± 0.54	kJ/mol	NIST Webbook
gf	74.82	kJ/mol	KDB
hcg	3343.31	kJ/mol	KDB
hcn	3123.230	kJ/mol	KDB
hf	-28.97	kJ/mol	KDB
hf	-25.50	kJ/mol	NIST Webbook
hfl	-51.60 ± 0.62	kJ/mol	NIST Webbook
hfus	3.90	kJ/mol	Joback Method
hvap	23.90	kJ/mol	NIST Webbook
ie	9.50 ± 0.10	eV	NIST Webbook
ie	9.53 ± 0.00	eV	NIST Webbook
ie	9.52	eV	NIST Webbook

ie	9.52 ± 0.01	eV	NIST Webbook
ie	9.52	eV	NIST Webbook
ie	9.51 ± 0.03	eV	NIST Webbook
ie	9.60 ± 0.03	eV	NIST Webbook
log10ws	-2.73		Aqueous Solubility Prediction Method
log10ws	-2.73		Estimated Solubility Method
logp	1.828		Crippen Method
mcvol	77.010	ml/mol	McGowan Method
nfpaf	%!d(float64=4)		KDB
nfpah	%!d(float64=2)		KDB
pc	3530.00	kPa	KDB
pc	3530.00 ± 30.00	kPa	NIST Webbook
rhoc	230.04 ± 2.10	kg/m3	NIST Webbook
rinpol	450.60		NIST Webbook
rinpol	450.00		NIST Webbook
rinpol	457.00		NIST Webbook
rinpol	450.20		NIST Webbook
rinpol	450.70		NIST Webbook
rinpol	449.80		NIST Webbook
rinpol	475.11		NIST Webbook
rinpol	451.00		NIST Webbook
rinpol	450.00		NIST Webbook
rinpol	471.10		NIST Webbook
rinpol	450.00		NIST Webbook
rinpol	457.00		NIST Webbook
rinpol	449.45		NIST Webbook
rinpol	472.00		NIST Webbook
rinpol	449.00		NIST Webbook
rinpol	450.00		NIST Webbook
rinpol	452.00		NIST Webbook
rinpol	452.00		NIST Webbook
rinpol	460.00		NIST Webbook
rinpol	454.00		NIST Webbook
rinpol	451.00		NIST Webbook
rinpol	450.00		NIST Webbook
rinpol	461.20		NIST Webbook
rinpol	462.00		NIST Webbook
rinpol	451.10		NIST Webbook
rinpol	445.14		NIST Webbook
rinpol	445.18		NIST Webbook
rinpol	445.00		NIST Webbook
rinpol	449.90		NIST Webbook
rinpol	450.00		NIST Webbook

rinpol	449.00		NIST Webbook
rinpol	473.00		NIST Webbook
rinpol	453.00		NIST Webbook
rinpol	458.00		NIST Webbook
rinpol	445.00		NIST Webbook
rinpol	457.00		NIST Webbook
rinpol	444.00		NIST Webbook
rinpol	450.00		NIST Webbook
rinpol	450.00		NIST Webbook
rinpol	451.00		NIST Webbook
rinpol	461.00		NIST Webbook
rinpol	455.00		NIST Webbook
rinpol	453.00		NIST Webbook
rinpol	457.00		NIST Webbook
rinpol	457.00		NIST Webbook
rinpol	459.00		NIST Webbook
rinpol	450.10		NIST Webbook
rinpol	452.00		NIST Webbook
rinpol	448.00		NIST Webbook
rinpol	457.10		NIST Webbook
ripol	490.00		NIST Webbook
ripol	487.00		NIST Webbook
sl	253.50	J/mol×K	NIST Webbook
sl	253.30	J/mol×K	NIST Webbook
tb	293.30	K	KDB
tc	452.70 ± 0.30	K	NIST Webbook
tc	451.38	K	Vapor Pressures and Vapor Liquid Critical Properties of Four Pentene Isomers
tc	452.70	K	KDB
tf	104.90	K	Aqueous Solubility Prediction Method
tf	104.70	K	KDB
tt	104.72 ± 0.02	K	NIST Webbook
tt	104.71 ± 0.05	K	NIST Webbook
tt	104.71 ± 0.02	K	NIST Webbook
vc	0.305	m3/kmol	NIST Webbook
vc	0.305	m3/kmol	KDB
zc	0.2859470		KDB
zra	0.27		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	153.67	J/mol×K	451.83	Joback Method
cpg	113.33	J/mol×K	310.04	Joback Method
cpg	122.05	J/mol×K	338.40	Joback Method
cpg	130.44	J/mol×K	366.76	Joback Method
cpg	138.50	J/mol×K	395.12	Joback Method
cpg	146.24	J/mol×K	423.47	Joback Method
cpg	160.80	J/mol×K	480.19	Joback Method
cpl	156.10	J/mol×K	298.15	NIST Webbook
cpl	156.06	J/mol×K	298.15	NIST Webbook
dvisc	0.0001932	Pa×s	310.04	Joback Method
dvisc	0.0003472	Pa×s	249.81	Joback Method
dvisc	0.0002509	Pa×s	279.93	Joback Method
dvisc	0.0005251	Pa×s	219.69	Joback Method
dvisc	0.0057693	Pa×s	129.35	Joback Method
dvisc	0.0019191	Pa×s	159.47	Joback Method
dvisc	0.0009056	Pa×s	189.58	Joback Method
hfust	5.36	kJ/mol	104.70	NIST Webbook
hfust	5.36	kJ/mol	104.71	NIST Webbook
hfust	5.36	kJ/mol	104.70	NIST Webbook
hfust	5.36	kJ/mol	104.71	NIST Webbook
hvapt	24.10	kJ/mol	293.30	KDB
hvapt	26.30	kJ/mol	280.50	NIST Webbook
hvapt	25.40	kJ/mol	298.50	NIST Webbook
rfi	1.36110		298.15	KDB
rhol	627.00	kg/m3	293.00	KDB
sfust	51.18	J/mol×K	104.71	NIST Webbook
sfust	51.18	J/mol×K	104.71	NIST Webbook
srf	0.01	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42164e+01
Coeff. B	-2.57363e+03

Coeff. C	-2.50700e+01
Temperature range (K), min.	209.84
Temperature range (K), max.	314.08

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.12332e+01
Coeff. B	-5.04579e+03
Coeff. C	-8.87493e+00
Coeff. D	1.15451e-05
Temperature range (K), min.	104.66
Temperature range (K), max.	450.37

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol194.mol
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Vapor Pressures and Vapor Liquid Critical Properties of Four Pentene Isomers:	https://www.doi.org/10.1021/acs.jced.7b00148
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=194
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C563451&Units=SI
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

Legend

af:	Acentric Factor
chl:	Standard liquid 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
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
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
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