1-Butene, 2-methyl-

Other names:	.gamma.-isoamylene
	1-isoamylene
	2-Methylbutene-1
	2-methyl-1-butene
	2-methylbut-1-ene
	C2H5C(CH3)=CH2
	Isopentene
	UN 2371
	UN 2459
	«gamma»-Isoamylene
Inchi:	InChI=1S/C5H10/c1-4-5(2)3/h2,4H2,1,3H3
InchiKey:	MHNNAWXXUZQSNM-UHFFFAOYSA-N
Formula:	C5H10
SMILES:	C=C(C)CC
Mol. weight [g/mol]:	70.13
CAS:	563-46-2

Physical Properties

Property code	Value	Unit	Source
af	0.2099		Cheméo Relay (1.0)
chl	-3335.74 ± 0.80	kJ/mol	NIST Webbook
gf	70.51	kJ/mol	Joback Method
hf	-34.80	kJ/mol	NIST Webbook
hf	-35.10 ± 0.84	kJ/mol	NIST Webbook
hfl	-60.96 ± 0.84	kJ/mol	NIST Webbook
hfus	6.12	kJ/mol	Joback Method
hvap	25.90 ± 0.10	kJ/mol	NIST Webbook
hvap	26.19	kJ/mol	NIST Webbook
hvap	25.90	kJ/mol	NIST Webbook
ie	9.12 ± 0.02	eV	NIST Webbook
ie	9.12 ± 0.01	eV	NIST Webbook
ie	9.10	eV	NIST Webbook
ie	9.15 ± 0.00	eV	NIST Webbook
ie	9.12	eV	NIST Webbook
ie	9.35 ± 0.08	eV	NIST Webbook
ie	9.12 ± 0.02	eV	NIST Webbook
ie	9.20 ± 0.10	eV	NIST Webbook

log10ws	-2.73		Estimated Solubility Method
log10ws	-2.73		Aqueous Solubility Prediction Method
logp	1.973		Crippen Method
mcvol	77.010	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
rinpol	489.00		NIST Webbook
rinpol	497.00		NIST Webbook
rinpol	500.00		NIST Webbook
rinpol	486.00		NIST Webbook
rinpol	488.00		NIST Webbook
rinpol	488.00		NIST Webbook
rinpol	490.00		NIST Webbook
rinpol	489.00		NIST Webbook
rinpol	497.00		NIST Webbook
rinpol	486.00		NIST Webbook
rinpol	499.00		NIST Webbook
rinpol	500.00		NIST Webbook
rinpol	496.80		NIST Webbook
rinpol	497.00		NIST Webbook
rinpol	494.40		NIST Webbook
rinpol	496.00		NIST Webbook
rinpol	493.58		NIST Webbook
rinpol	493.79		NIST Webbook
rinpol	494.00		NIST Webbook
rinpol	487.80		NIST Webbook
rinpol	523.00		NIST Webbook
rinpol	488.00		NIST Webbook
rinpol	488.00		NIST Webbook
rinpol	506.00		NIST Webbook
rinpol	495.00		NIST Webbook
rinpol	496.00		NIST Webbook
rinpol	480.00		NIST Webbook
rinpol	495.00		NIST Webbook
rinpol	493.00		NIST Webbook
rinpol	493.00		NIST Webbook
rinpol	495.00		NIST Webbook
rinpol	493.00		NIST Webbook
rinpol	489.00		NIST Webbook
rinpol	496.00		NIST Webbook
rinpol	488.00		NIST Webbook
rinpol	500.00		NIST Webbook
rinpol	494.00		NIST Webbook
rinpol	496.00		NIST Webbook

rinpol	494.00		NIST Webbook
rinpol	493.00		NIST Webbook
rinpol	487.00		NIST Webbook
rinpol	493.00		NIST Webbook
rinpol	487.00		NIST Webbook
rinpol	489.00		NIST Webbook
rinpol	496.00		NIST Webbook
rinpol	487.00		NIST Webbook
rinpol	496.80		NIST Webbook
rinpol	487.00		NIST Webbook
rinpol	487.63		NIST Webbook
rinpol	495.60		NIST Webbook
rinpol	488.20		NIST Webbook
rinpol	488.00		NIST Webbook
rinpol	490.00		NIST Webbook
rinpol	488.00		NIST Webbook
rinpol	491.00		NIST Webbook
rinpol	495.00		NIST Webbook
rinpol	495.00		NIST Webbook
rinpol	494.00		NIST Webbook
rinpol	493.00		NIST Webbook
rinpol	488.00		NIST Webbook
rinpol	488.00		NIST Webbook
rinpol	488.48		NIST Webbook
rinpol	488.20		NIST Webbook
rinpol	488.10		NIST Webbook
rinpol	487.90		NIST Webbook
ripol	545.00		NIST Webbook
ripol	534.00		NIST Webbook
ripol	575.00		NIST Webbook
ripol	575.00		NIST Webbook
sl	253.97	J/mol×K	NIST Webbook
sl	254.00	J/mol×K	NIST Webbook
tb	304.10 ± 0.50	K	NIST Webbook
tb	304.20 ± 0.30	K	NIST Webbook
tb	304.05 ± 1.00	K	NIST Webbook
tb	304.15 ± 0.30	K	NIST Webbook
tb	304.20 ± 0.15	K	NIST Webbook
tb	304.20 ± 0.20	K	NIST Webbook
tb	305.10 ± 1.50	K	NIST Webbook
tb	304.50 ± 1.00	K	NIST Webbook
tb	303.65 ± 2.00	K	NIST Webbook
tb	305.00 ± 3.00	K	NIST Webbook
tb	311.00 ± 2.00	K	NIST Webbook

tb	303.45 ± 3.00	K	NIST Webbook
tb	304.15 ± 2.00	K	NIST Webbook
tb	307.15 ± 2.00	K	NIST Webbook
tb	306.15 ± 2.00	K	NIST Webbook
tb	305.15 ± 2.00	K	NIST Webbook
tb	304.65 ± 2.00	K	NIST Webbook
tb	304.40	K	NIST Webbook
tb	304.30	K	NIST Webbook
tb	304.27 ± 0.30	K	NIST Webbook
tb	304.40 ± 0.30	K	NIST Webbook
tb	304.20 ± 0.60	K	NIST Webbook
tb	304.31 ± 0.30	K	NIST Webbook
tb	303.50 ± 2.50	K	NIST Webbook
tb	304.50 ± 2.00	K	NIST Webbook
tb	304.20 ± 0.40	K	NIST Webbook
tb	304.20 ± 1.00	K	NIST Webbook
tb	304.30 ± 0.30	K	NIST Webbook
tb	304.15 ± 1.00	K	NIST Webbook
tb	304.20 ± 0.15	K	NIST Webbook
tb	304.27 ± 0.40	K	NIST Webbook
tb	304.20 ± 0.30	K	NIST Webbook
tb	304.20 ± 0.40	K	NIST Webbook
tb	304.15 ± 1.00	K	NIST Webbook
tb	304.60 ± 0.50	K	NIST Webbook
tb	304.05 ± 0.50	K	NIST Webbook
tb	304.65 ± 0.50	K	NIST Webbook
tb	304.35 ± 0.50	K	NIST Webbook
tc	467.00	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tc	470.00	K	NIST Webbook
tc	467.90	K	Vapor Pressures and Vapor Liquid Critical Properties of Four Pentene Isomers
tf	135.59 ± 0.03	K	NIST Webbook
tf	135.56 ± 0.05	K	NIST Webbook
tf	134.97 ± 0.40	K	NIST Webbook
tf	135.56 ± 0.06	K	NIST Webbook
tf	135.77	K	Aqueous Solubility Prediction Method
tf	138.95 ± 0.30	K	NIST Webbook
tf	135.09 ± 0.30	K	NIST Webbook
tt	135.62 ± 0.02	K	NIST Webbook
tt	135.60 ± 0.02	K	NIST Webbook
tt	135.62 ± 0.02	K	NIST Webbook

tt	135.60 ± 0.02	K	NIST Webbook
vc	0.288	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	116.15 ± 0.35	J/mol×K	320.66	NIST Webbook
cpg	165.35 ± 0.50	J/mol×K	502.21	NIST Webbook
cpg	153.13 ± 0.46	J/mol×K	453.41	NIST Webbook
cpg	140.62 ± 0.42	J/mol×K	407.11	NIST Webbook
cpg	128.37 ± 0.39	J/mol×K	362.51	NIST Webbook
cpl	157.30	J/mol×K	298.15	NIST Webbook
cpl	157.19	J/mol×K	298.15	NIST Webbook
hfust	7.91	kJ/mol	135.60	NIST Webbook
hfust	7.91	kJ/mol	135.62	NIST Webbook
hfust	5.36	kJ/mol	104.70	NIST Webbook
hfust	7.91	kJ/mol	135.62	NIST Webbook
hfust	7.91	kJ/mol	135.60	NIST Webbook
hfust	7.91	kJ/mol	135.60	NIST Webbook
hvapt	25.50	kJ/mol	304.30	NIST Webbook
hvapt	28.50	kJ/mol	288.00	NIST Webbook
hvapt	27.30	kJ/mol	305.00	NIST Webbook
hvapt	25.50 ± 0.10	kJ/mol	304.00	NIST Webbook
sfust	58.33	J/mol×K	135.62	NIST Webbook
sfust	58.34	J/mol×K	135.60	NIST Webbook
sfust	58.34	J/mol×K	135.60	NIST Webbook
sfust	58.33	J/mol×K	135.62	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.78967e+01
Coeff. B	-5.23519e+03
Coeff. C	-8.20067e+00
Coeff. D	8.78420e-06
Temperature range (K), min.	135.58

Temperature range (K), max.	465.00

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol193.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C563462&Units=SI
Vapor Pressures and Vapor Liquid Critical Properties of Four Pentene Isomers:	https://www.doi.org/10.1021/acs.jced.7b00148
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons:	https://www.doi.org/10.1021/je0341357
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Cheméo Relay (1.0, beta):	
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=193

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
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume