2-Butene, 2-methyl-

Other names:	(CH3)2C=CHCH3
	1,1,2-TRIMETHYLETHYLENE
	2-Methy-2-Butene
	2-Methyl-2-butene
	2-Methylbut-2-ene
	2-Methylbutene-2
	3-METHYL-2-BUTENE
	AMYLENE
	Ethylene, trimethyl-
	NSC 74118
	Trimethylethylene
	UN 2460
	b-isoamylene
	n-Amylene
	«beta»-Isoamylene
	Â«betaÂ»-Isoamylene
Inchi:	InChI=1S/C5H10/c1-4-5(2)3/h4H,1-3H3
InchiKey:	BKOOMYPCSUNDGP-UHFFFAOYSA-N
Formula:	C5H10
SMILES:	CC=C(C)C
Mol. weight [g/mol]:	70.13
CAS:	513-35-9

Physical Properties

Property code	Value	Unit	Source
af	0.2440		KDB
affp	808.80	kJ/mol	NIST Webbook
ap	285.950	K	KDB
basg	779.90	kJ/mol	NIST Webbook
chl	-3328.60 ± 1.30	kJ/mol	NIST Webbook
gf	59.70	kJ/mol	KDB
hcg	3326.91	kJ/mol	KDB
hcn	3106.829	kJ/mol	KDB
hf	-42.58	kJ/mol	KDB
hf	-41.50 ± 0.88	kJ/mol	NIST Webbook
hf	-41.00	kJ/mol	NIST Webbook
hfl	-68.60 ± 0.80	kJ/mol	NIST Webbook

hfl	-68.10 ± 1.30	kJ/mol	NIST Webbook
hfus	7.60	kJ/mol	Joback Method
hvap	27.10 ± 0.10	kJ/mol	NIST Webbook
hvap	27.34	kJ/mol	NIST Webbook
hvap	27.10	kJ/mol	NIST Webbook
ie	8.72	eV	NIST Webbook
ie	8.67 ± 0.02	eV	NIST Webbook
ie	8.68	eV	NIST Webbook
ie	8.85 ± 0.04	eV	NIST Webbook
ie	8.69 ± 0.01	eV	NIST Webbook
ie	8.69	eV	NIST Webbook
ie	8.68 ± 0.02	eV	NIST Webbook
ie	8.68 ± 0.00	eV	NIST Webbook
ie	8.70	eV	NIST Webbook
ie	8.83 ± 0.11	eV	NIST Webbook
log10ws	-2.56		Estimated Solubility Method
log10ws	-2.56		Aqueous Solubility Prediction Method
logp	1.973		Crippen Method
mcvol	77.010	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
pc	3420.00	kPa	KDB
pc	3420.00 ± 100.00	kPa	NIST Webbook
rinpol	519.00		NIST Webbook
rinpol	514.00		NIST Webbook
rinpol	517.00		NIST Webbook
rinpol	524.00		NIST Webbook
rinpol	517.00		NIST Webbook
rinpol	523.00		NIST Webbook
rinpol	520.00		NIST Webbook
rinpol	520.00		NIST Webbook
rinpol	517.00		NIST Webbook
rinpol	517.00		NIST Webbook
rinpol	514.00		NIST Webbook
rinpol	520.20		NIST Webbook
rinpol	513.80		NIST Webbook
rinpol	515.00		NIST Webbook
rinpol	520.10		NIST Webbook
rinpol	504.00		NIST Webbook
rinpol	504.00		NIST Webbook
rinpol	520.00		NIST Webbook
rinpol	519.80		NIST Webbook
rinpol	520.00		NIST Webbook

rinpol	519.80	NIST Webbook
rinpol	514.30	NIST Webbook
rinpol	514.40	NIST Webbook
rinpol	523.00	NIST Webbook
rinpol	519.00	NIST Webbook
rinpol	525.00	NIST Webbook
rinpol	520.00	NIST Webbook
rinpol	520.00	NIST Webbook
rinpol	520.00	NIST Webbook
rinpol	514.50	NIST Webbook
rinpol	519.90	NIST Webbook
rinpol	520.30	NIST Webbook
rinpol	514.50	NIST Webbook
rinpol	514.70	NIST Webbook
rinpol	514.00	NIST Webbook
rinpol	520.00	NIST Webbook
rinpol	520.00	NIST Webbook
rinpol	520.00	NIST Webbook
rinpol	519.00	NIST Webbook
rinpol	514.33	NIST Webbook
rinpol	514.00	NIST Webbook
rinpol	514.00	NIST Webbook
rinpol	526.00	NIST Webbook
rinpol	514.00	NIST Webbook
rinpol	514.00	NIST Webbook
rinpol	513.75	NIST Webbook
rinpol	514.00	NIST Webbook
rinpol	507.00	NIST Webbook
rinpol	514.00	NIST Webbook
rinpol	514.00	NIST Webbook
rinpol	515.00	NIST Webbook
rinpol	515.00	NIST Webbook
rinpol	515.00	NIST Webbook
rinpol	515.00	NIST Webbook
rinpol	522.00	NIST Webbook
rinpol	514.00	NIST Webbook
rinpol	526.00	NIST Webbook
rinpol	527.00	NIST Webbook
rinpol	525.00	NIST Webbook
rinpol	523.00	NIST Webbook
rinpol	515.80	NIST Webbook
rinpol	518.60	NIST Webbook
rinpol	520.00	NIST Webbook
rinpol	513.84	NIST Webbook

rinpol	514.38		NIST Webbook
rinpol	514.00		NIST Webbook
rinpol	520.30		NIST Webbook
rinpol	519.50		NIST Webbook
rinpol	520.40		NIST Webbook
rinpol	514.20		NIST Webbook
rinpol	530.00		NIST Webbook
rinpol	514.00		NIST Webbook
rinpol	515.00		NIST Webbook
rinpol	531.00		NIST Webbook
rinpol	519.00		NIST Webbook
rinpol	521.00		NIST Webbook
rinpol	498.00		NIST Webbook
rinpol	514.00		NIST Webbook
rinpol	522.00		NIST Webbook
rinpol	522.00		NIST Webbook
rinpol	519.00		NIST Webbook
rinpol	515.00		NIST Webbook
rinpol	502.00		NIST Webbook
rinpol	515.00		NIST Webbook
rinpol	521.00		NIST Webbook
rinpol	514.00		NIST Webbook
rinpol	515.00		NIST Webbook
ripol	614.00		NIST Webbook
ripol	561.00		NIST Webbook
ripol	573.00		NIST Webbook
ripol	614.00		NIST Webbook
sl	251.04	J/mol×K	NIST Webbook
sl	251.20	J/mol×K	NIST Webbook
sl	248.90	J/mol×K	NIST Webbook
tb	311.71	K	KDB
tc	481.00	K	NIST Webbook
tc	470.00 ± 1.00	K	NIST Webbook
tc	477.47	K	Vapor Pressures and Vapor Liquid Critical Properties of Four Pentene Isomers
tc	470.00	K	KDB
tf	150.00 ± 4.00	K	NIST Webbook
tf	139.39	K	KDB
tf	139.22	K	Aqueous Solubility Prediction Method
tf	146.00 ± 6.00	K	NIST Webbook
tf	139.35 ± 0.04	K	NIST Webbook
tf	139.37 ± 0.02	K	NIST Webbook
tf	139.12 ± 0.40	K	NIST Webbook

tf	140.20 ± 0.50	K	NIST Webbook
tf	139.00 ± 1.50	K	NIST Webbook
tf	139.00 ± 1.00	K	NIST Webbook
tf	127.10 ± 0.70	K	NIST Webbook
tf	139.35 ± 0.07	K	NIST Webbook
tt	139.40 ± 0.02	K	NIST Webbook
tt	139.42 ± 0.05	K	NIST Webbook
tt	139.44 ± 0.60	K	NIST Webbook
tt	139.42 ± 0.60	K	NIST Webbook
tt	138.90 ± 0.20	K	NIST Webbook
vc	0.296	m3/kmol	Joback Method
zra	0.26		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.05 ± 0.46	J/mol×K	471.09	NIST Webbook
cpg	143.05 ± 0.43	J/mol×K	436.18	NIST Webbook
cpg	133.93 ± 0.40	J/mol×K	402.26	NIST Webbook
cpg	122.97 ± 0.37	J/mol×K	362.37	NIST Webbook
cpg	111.00 ± 0.33	J/mol×K	319.04	NIST Webbook
cpl	152.80	J/mol×K	298.15	NIST Webbook
cpl	146.40	J/mol×K	293.90	NIST Webbook
cpl	152.80	J/mol×K	298.15	NIST Webbook
hfust	7.60	kJ/mol	139.40	NIST Webbook
hfust	7.60	kJ/mol	139.42	NIST Webbook
hfust	7.59	kJ/mol	139.40	NIST Webbook
hfust	7.43	kJ/mol	138.90	NIST Webbook
hfust	7.58	kJ/mol	139.40	NIST Webbook
hvapt	28.30	kJ/mol	310.00	NIST Webbook
hvapt	27.50 ± 0.10	kJ/mol	290.00	NIST Webbook
hvapt	26.31	kJ/mol	311.70	NIST Webbook
hvapt	28.40	kJ/mol	307.00	NIST Webbook
hvapt	26.30	kJ/mol	311.70	KDB
hvapt	26.30 ± 0.10	kJ/mol	312.00	NIST Webbook
rfi	1.38760		293.15	Isobaric Vapor Liquid Equilibrium for Nine Binary Systems of Cracking C5 Fraction at 250 kPa

rfi	1.38420		298.15	KDB
rhol	662.00	kg/m3	293.00	KDB
sfust	5.35	J/mol×K	138.90	NIST Webbook
sfust	54.49	J/mol×K	139.42	NIST Webbook
sfust	54.37	J/mol×K	139.40	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	1.43288e+01
Coeff. B	-2.72849e+03
Coeff. C	-3.07250e+01
Temperature range (K), min.	225.05
Temperature range (K), max.	333.31

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.56700e+01
Coeff. B	-5.58161e+03
Coeff. C	-9.44186e+00
Coeff. D	1.09937e-05
Temperature range (K), min.	139.39
Temperature range (K), max.	471.00

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=195

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C513359&Units=SI

Thermochemistry of Benzyl Alcohol: https://www.doi.org/10.1021/je049823k

Reaction Equilibria Involving Benzyl Alcohol and tert-Alkyl Ethers:

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Isobaric Vapor Liquid Equilibrium for Nine Binary Systems of Cracking C5 Fraction at 250 kPa: https://www.doi.org/10.1021/acs.jced.6b00180

Thermochemistry of Branched Ethers: https://www.doi.org/10.1021/je034172y

Experimental Study of Chemical Equilibrium in the Reacting System of tert-Amyl Alkyl Ether Synthesis:

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Vapor Pressures and Vapor Liquid Critical Properties of Four Pentene Isomers:	https://www.doi.org/10.1021/acs.jced.7b00148
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol195.mol

Legend

af:	Acentric Factor
affp:	Proton affinity
ap:	Aniline Point
basg:	Gas basicity
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
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
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
zra:	Rackett Parameter