2-Butene, 2,3-dimethyl-

Other names: (CH3)2C=C(CH3)2
1,1,2,2-TETRAMETHYLETHYLENE
2,3-Dimethyl-2-butene
2,3-Dimethylbut-2-ene
2,3-Dimethylbutene-2
TETRAMETHYLETHYLENE
Tetramethylethene

Inchi: InChI=1S/C6H12/c1-5(2)6(3)4/h1-4H3

InchiKey: WGLLSSPDPJPLOR-UHFFFAOYSA-N

Formula: C6H12

SMILES: CC(C)=C(C)C

Mol. weight [g/mol]: 84.16

CAS: 563-79-1

Physical Properties

Property code	Value	Unit	Source
af	0.2390		KDB
affp	813.90	kJ/mol	NIST Webbook
basg	785.90	kJ/mol	NIST Webbook
gf	75.91	kJ/mol	KDB
hcg	3974.72	kJ/mol	KDB
hcn	3710.622	kJ/mol	KDB
hf	-69.84	kJ/mol	KDB
hf	-70.30 ± 1.50	kJ/mol	NIST Webbook
hf	-68.40 ± 1.50	kJ/mol	NIST Webbook
hfl	-102.90 ± 1.50	kJ/mol	NIST Webbook
hfus	8.88	kJ/mol	Joback Method
hvap	32.50	kJ/mol	NIST Webbook
hvap	32.60	kJ/mol	NIST Webbook
hvap	32.60	kJ/mol	NIST Webbook
hvap	32.67	kJ/mol	NIST Webbook
ie	8.16	eV	NIST Webbook
ie	8.46	eV	NIST Webbook
ie	8.42	eV	NIST Webbook
ie	8.30	eV	NIST Webbook
ie	10.52	eV	NIST Webbook
ie	8.30	eV	NIST Webbook

ie	8.27 ± 0.01	eV	NIST Webbook
ie	8.26	eV	NIST Webbook
ie	8.27 ± 0.01	eV	NIST Webbook
ie	8.27 ± 0.02	eV	NIST Webbook
log10ws	-2.19		Crippen Method
logp	2.363		Crippen Method
mcvol	91.100	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
pc	3360.00	kPa	KDB
rinpol	627.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	624.20		NIST Webbook
rinpol	632.00		NIST Webbook
rinpol	624.38		NIST Webbook
rinpol	624.32		NIST Webbook
rinpol	624.00		NIST Webbook
rinpol	632.00		NIST Webbook
rinpol	612.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	627.00		NIST Webbook
rinpol	649.00		NIST Webbook
rinpol	624.00		NIST Webbook
rinpol	627.00		NIST Webbook
rinpol	624.20		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	627.00		NIST Webbook
rinpol	630.40		NIST Webbook
rinpol	624.20		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	631.00		NIST Webbook
rinpol	631.00		NIST Webbook
rinpol	630.60		NIST Webbook
rinpol	631.10		NIST Webbook
rinpol	625.30		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	631.00		NIST Webbook
rinpol	631.00		NIST Webbook
rinpol	624.80		NIST Webbook

rinpol	626.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	631.00		NIST Webbook
sl	272.40	J/mol×K	NIST Webbook
sl	270.20	J/mol×K	NIST Webbook
tb	346.40	K	KDB
tb	346.15	K	Isobaric vapor-liquid equilibrium for systems containing sulfur compounds
tb	346.15	K	Isobaric vapor-liquid equilibrium for four binary systems of 3-methylthiophene
tb	346.15	K	Isobaric vapor-liquid equilibrium for four binary systems of thiophene
tc	524.00	K	NIST Webbook
tc	524.00	K	KDB
tc	521.00	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tf	198.61 ± 0.30	K	NIST Webbook
tf	198.87 ± 0.03	K	NIST Webbook
tf	197.75 ± 0.20	K	NIST Webbook
tf	198.82 ± 0.06	K	NIST Webbook
tf	198.30 ± 0.60	K	NIST Webbook
tf	198.88 ± 0.02	K	NIST Webbook
tf	199.00 ± 0.50	K	NIST Webbook
tf	198.86 ± 0.05	K	NIST Webbook
tf	198.90	K	KDB
tf	198.61 ± 0.50	K	NIST Webbook
tf	198.85 ± 0.15	K	NIST Webbook
tf	198.61 ± 0.30	K	NIST Webbook
tf	196.75 ± 0.60	K	NIST Webbook
tf	198.84 ± 0.04	K	NIST Webbook
tf	198.87 ± 0.03	K	NIST Webbook
tf	198.82 ± 0.20	K	NIST Webbook
tt	198.90 ± 0.05	K	NIST Webbook

tt	198.92 ± 0.02	K	NIST Webbook
tt	198.50 ± 0.20	K	NIST Webbook
tt	198.92 ± 0.01	K	NIST Webbook
vc	0.351	m3/kmol	KDB
zc	0.2706940		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.33 ± 0.36	J/mol×K	473.20	NIST Webbook
cpg	167.65 ± 0.34	J/mol×K	433.20	NIST Webbook
cpg	142.00 ± 0.28	J/mol×K	355.25	NIST Webbook
cpg	154.64 ± 0.31	J/mol×K	393.20	NIST Webbook
cpg	135.31 ± 0.27	J/mol×K	334.20	NIST Webbook
cpl	175.73	J/mol×K	295.50	NIST Webbook
cpl	174.68	J/mol×K	298.15	NIST Webbook
hfust	6.44	kJ/mol	198.90	NIST Webbook
hfust	6.44	kJ/mol	198.90	NIST Webbook
hfust	3.53	kJ/mol	196.80	NIST Webbook
hvapt	32.70	kJ/mol	318.00	NIST Webbook
hvapt	32.00 ± 0.10	kJ/mol	308.00	NIST Webbook
hvapt	32.90 ± 0.10	kJ/mol	292.00	NIST Webbook
hvapt	32.10	kJ/mol	329.50	NIST Webbook
hvapt	29.70 ± 0.10	kJ/mol	346.00	NIST Webbook
hvapt	33.10	kJ/mol	315.00	NIST Webbook
hvapt	29.64	kJ/mol	346.40	NIST Webbook
hvapt	29.64	kJ/mol	346.40	KDB
hvapt	30.90 ± 0.10	kJ/mol	326.00	NIST Webbook
pvap	38.40	kPa	318.44	Isobaric Vapor Liquid Equilibrium for 2,3-Dimethyl-2-butene + Methanol, + Ethanol, + 2-Propanol, or + 2-Butanol at Atmospheric Pressure
pvap	271.20	kPa	381.62	Isothermal vapor-liquid equilibria for methanol and 2,3-dimethyl-2-butene at 343.15 K, 353.15 K, 363.15 K, 373.15 K

pvap	281.30	kPa	383.05	Isothermal vapor-liquid equilibria for methanol and 2,3-dimethyl-2-butene at 343.15 K, 353.15 K, 363.15 K, 373.15 K
pvap	292.10	kPa	384.70	Isothermal vapor-liquid equilibria for methanol and 2,3-dimethyl-2-butene at 343.15 K, 353.15 K, 363.15 K, 373.15 K
pvap	306.80	kPa	386.65	Isothermal vapor-liquid equilibria for methanol and 2,3-dimethyl-2-butene at 343.15 K, 353.15 K, 363.15 K, 373.15 K
pvap	318.40	kPa	388.20	Isothermal vapor-liquid equilibria for methanol and 2,3-dimethyl-2-butene at 343.15 K, 353.15 K, 363.15 K, 373.15 K
pvap	30.29	kPa	312.39	Isobaric Vapor Liquid Equilibrium for 2,3-Dimethyl-2-butene + Methanol, + Ethanol, + 2-Propanol, or + 2-Butanol at Atmospheric Pressure
pvap	255.10	kPa	379.15	Isothermal vapor-liquid equilibria for methanol and 2,3-dimethyl-2-butene at 343.15 K, 353.15 K, 363.15 K, 373.15 K
pvap	47.72	kPa	324.24	Isobaric Vapor Liquid Equilibrium for 2,3-Dimethyl-2-butene + Methanol, + Ethanol, + 2-Propanol, or + 2-Butanol at Atmospheric Pressure

pvap	54.12	kPa	327.70	Isobaric Vapor Liquid Equilibrium for 2,3-Dimethyl-2-butene + Methanol, + Ethanol, + 2-Propanol, or + 2-Butanol at Atmospheric Pressure
pvap	59.32	kPa	330.28	Isobaric Vapor Liquid Equilibrium for 2,3-Dimethyl-2-butene + Methanol, + Ethanol, + 2-Propanol, or + 2-Butanol at Atmospheric Pressure
pvap	230.40	kPa	375.20	Isothermal vapor-liquid equilibria for methanol and 2,3-dimethyl-2-butene at 343.15 K, 353.15 K, 363.15 K, 373.15 K
pvap	75.19	kPa	337.15	Isobaric Vapor Liquid Equilibrium for 2,3-Dimethyl-2-butene + Methanol, + Ethanol, + 2-Propanol, or + 2-Butanol at Atmospheric Pressure
pvap	80.30	kPa	339.12	Isobaric Vapor Liquid Equilibrium for 2,3-Dimethyl-2-butene + Methanol, + Ethanol, + 2-Propanol, or + 2-Butanol at Atmospheric Pressure
pvap	85.40	kPa	340.98	Isobaric Vapor Liquid Equilibrium for 2,3-Dimethyl-2-butene + Methanol, + Ethanol, + 2-Propanol, or + 2-Butanol at Atmospheric Pressure

pvap	90.74	kPa	342.81	Isobaric Vapor Liquid Equilibrium for 2,3-Dimethyl-2-butene + Methanol, + Ethanol, + 2-Propanol, or + 2-Butanol at Atmospheric Pressure
pvap	94.64	kPa	344.13	Isobaric Vapor Liquid Equilibrium for 2,3-Dimethyl-2-butene + Methanol, + Ethanol, + 2-Propanol, or + 2-Butanol at Atmospheric Pressure
pvap	101.43	kPa	346.28	Isobaric Vapor Liquid Equilibrium for 2,3-Dimethyl-2-butene + Methanol, + Ethanol, + 2-Propanol, or + 2-Butanol at Atmospheric Pressure
pvap	218.80	kPa	373.18	Isothermal vapor-liquid equilibria for methanol and 2,3-dimethyl-2-butene at 343.15 K, 353.15 K, 363.15 K, 373.15 K
pvap	202.80	kPa	370.36	Isothermal vapor-liquid equilibria for methanol and 2,3-dimethyl-2-butene at 343.15 K, 353.15 K, 363.15 K, 373.15 K
pvap	190.90	kPa	368.05	Isothermal vapor-liquid equilibria for methanol and 2,3-dimethyl-2-butene at 343.15 K, 353.15 K, 363.15 K, 373.15 K
pvap	179.50	kPa	365.76	Isothermal vapor-liquid equilibria for methanol and 2,3-dimethyl-2-butene at 343.15 K, 353.15 K, 363.15 K, 373.15 K

pvap	164.80	kPa	362.80	Isothermal vapor-liquid equilibria for methanol and 2,3-dimethyl-2-butene at 343.15 K, 353.15 K, 363.15 K, 373.15 K
pvap	140.40	kPa	357.22	Isothermal vapor-liquid equilibria for methanol and 2,3-dimethyl-2-butene at 343.15 K, 353.15 K, 363.15 K, 373.15 K
pvap	133.30	kPa	355.35	Isothermal vapor-liquid equilibria for methanol and 2,3-dimethyl-2-butene at 343.15 K, 353.15 K, 363.15 K, 373.15 K
pvap	125.50	kPa	353.46	Isothermal vapor-liquid equilibria for methanol and 2,3-dimethyl-2-butene at 343.15 K, 353.15 K, 363.15 K, 373.15 K
pvap	113.90	kPa	350.10	Isothermal vapor-liquid equilibria for methanol and 2,3-dimethyl-2-butene at 343.15 K, 353.15 K, 363.15 K, 373.15 K
pvap	105.30	kPa	347.65	Isothermal vapor-liquid equilibria for methanol and 2,3-dimethyl-2-butene at 343.15 K, 353.15 K, 363.15 K, 373.15 K
pvap	94.70	kPa	344.20	Isothermal vapor-liquid equilibria for methanol and 2,3-dimethyl-2-butene at 343.15 K, 353.15 K, 363.15 K, 373.15 K

pvap	90.20	kPa	342.65	Isothermal vapor-liquid equilibria for methanol and 2,3-dimethyl-2-butene at 343.15 K, 353.15 K, 363.15 K, 373.15 K
pvap	84.20	kPa	340.60	Isothermal vapor-liquid equilibria for methanol and 2,3-dimethyl-2-butene at 343.15 K, 353.15 K, 363.15 K, 373.15 K
pvap	77.50	kPa	338.20	Isothermal vapor-liquid equilibria for methanol and 2,3-dimethyl-2-butene at 343.15 K, 353.15 K, 363.15 K, 373.15 K
pvap	73.50	kPa	336.50	Isothermal vapor-liquid equilibria for methanol and 2,3-dimethyl-2-butene at 343.15 K, 353.15 K, 363.15 K, 373.15 K
pvap	101.20	kPa	346.24	Isothermal vapor-liquid equilibria for methanol and 2,3-dimethyl-2-butene at 343.15 K, 353.15 K, 363.15 K, 373.15 K
pvap	65.23	kPa	333.00	Isobaric Vapor Liquid Equilibrium for 2,3-Dimethyl-2-butene + Methanol, + Ethanol, + 2-Propanol, or + 2-Butanol at Atmospheric Pressure
pvap	238.50	kPa	376.50	Isothermal vapor-liquid equilibria for methanol and 2,3-dimethyl-2-butene at 343.15 K, 353.15 K, 363.15 K, 373.15 K
rfi	1.40952		298.15	KDB
rhol	708.00	kg/m3	293.00	KDB
sfust	17.94	J/mol×K	196.80	NIST Webbook
sfust	32.39	J/mol×K	198.90	NIST Webbook

srf	0.02	N/m	298.20	KDB
tcondl	0.12	W/m×K	294.09	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.11	W/m×K	326.77	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.11	W/m×K	327.02	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.11	W/m×K	326.42	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	294.63	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.12	W/m×K	294.40	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.11	W/m×K	322.98	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.13	W/m×K	278.72	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.13	W/m×K	278.50	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.13	W/m×K	278.21	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	

tcondl	0.14	W/m×K	259.37	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.14	W/m×K	259.17	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.14	W/m×K	258.89	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.11	W/m×K	322.74	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.11	W/m×K	322.40	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.12	W/m×K	313.34	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.12	W/m×K	313.09	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.12	W/m×K	312.76	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38453e+01
Coeff. B	-2.75751e+03
Coeff. C	-4.74970e+01
Temperature range (K), min.	250.89
Temperature range (K), max.	370.62

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2

Coeff. A	6.73770e+01
Coeff. B	-6.03585e+03
Coeff. C	-7.86074e+00
Coeff. D	5.28509e-06
Temperature range (K), min.	198.92
Temperature range (K), max.	524.00

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/files/research/kdb/mol/mol212.mol
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=212
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C563791&Units=SI
Isothermal vapor-liquid equilibria for methanol and 2,3-dimethyl-2-butene at 348.15 K, 353.15 K, 363.15 K, 373.15 K:	https://www.doi.org/10.1016/j.fluid.2011.07.014
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Isobaric Vapor Liquid Equilibrium for 2,3-Dimethyl-2-butene + Methanol, + Ethanol, + 2-Propanol, or + 2-Butanol at Atmospheric Pressure:	https://www.doi.org/10.1021/je034106w
Isobaric vapor-liquid equilibrium for systems containing sulfur compounds:	https://www.doi.org/10.1016/j.fluid.2013.05.019
Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons:	https://www.doi.org/10.1021/je0341357
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Isobaric vapor-liquid equilibrium for four binary systems of thiophene:	https://www.doi.org/10.1016/j.fluid.2011.11.020
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=212
Isobaric vapor-liquid equilibrium for four binary systems of 3-methylthiophene:	https://www.doi.org/10.1016/j.fluid.2012.02.005
Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids:	https://www.doi.org/10.1021/je034162x
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons:	

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
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
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-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
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility