1-Butene, 2,3-dimethyl-

Other names:	(CH3)2CHC(CH3)=CH2
	2,3-Dimethyl-1-butene
	2,3-Dimethylbutene-1
	2,3-dimethylbut-1-ene
Inchi:	InChI=1S/C6H12/c1-5(2)6(3)4/h6H,1H2,2-4H3
InchiKey:	OWWIWYDDISJUMY-UHFFFAOYSA-N
Formula:	C6H12
SMILES:	C=C(C)C(C)C
Mol. weight [g/mol]:	84.16
CAS:	563-78-0

Physical Properties

Property code	Value	Unit	Source
af	0.2210		KDB
gf	79.09	kJ/mol	KDB
hcg	3981.95	kJ/mol	KDB
hcn	3717.861	kJ/mol	KDB
hf	-66.36	kJ/mol	KDB
hf	-61.00 ± 2.00	kJ/mol	NIST Webbook
hf	-65.90 ± 1.50	kJ/mol	NIST Webbook
hfl	-95.10 ± 1.50	kJ/mol	NIST Webbook
hfus	5.18	kJ/mol	Joback Method
hvap	29.20	kJ/mol	NIST Webbook
hvap	29.20	kJ/mol	NIST Webbook
hvap	29.20	kJ/mol	NIST Webbook
ie	9.07 ± 0.02	eV	NIST Webbook
ie	9.07 ± 0.01	eV	NIST Webbook
ie	9.07 ± 0.01	eV	NIST Webbook
ie	8.41	eV	NIST Webbook
log10ws	-1.95		Crippen Method
logp	2.219		Crippen Method
mcvol	91.100	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
pc	3240.00	kPa	KDB
rinpol	561.00		NIST Webbook
rinpol	562.00		NIST Webbook
rinpol	571.00		NIST Webbook

rinpol	570.00	NIST Webbook
rinpol	566.00	NIST Webbook
rinpol	560.00	NIST Webbook
rinpol	566.10	NIST Webbook
rinpol	564.00	NIST Webbook
rinpol	548.00	NIST Webbook
rinpol	564.00	NIST Webbook
rinpol	567.00	NIST Webbook
rinpol	559.60	NIST Webbook
rinpol	560.00	NIST Webbook
rinpol	557.39	NIST Webbook
rinpol	566.00	NIST Webbook
rinpol	568.00	NIST Webbook
rinpol	558.00	NIST Webbook
rinpol	554.00	NIST Webbook
rinpol	558.30	NIST Webbook
rinpol	555.90	NIST Webbook
rinpol	557.00	NIST Webbook
rinpol	564.90	NIST Webbook
rinpol	569.00	NIST Webbook
rinpol	572.50	NIST Webbook
rinpol	559.00	NIST Webbook
rinpol	558.30	NIST Webbook
rinpol	566.10	NIST Webbook
rinpol	557.60	NIST Webbook
rinpol	557.00	NIST Webbook
rinpol	566.00	NIST Webbook
rinpol	566.00	NIST Webbook
rinpol	567.00	NIST Webbook
rinpol	560.00	NIST Webbook
rinpol	565.80	NIST Webbook
rinpol	566.30	NIST Webbook
rinpol	558.80	NIST Webbook
rinpol	559.60	NIST Webbook
rinpol	566.00	NIST Webbook
rinpol	566.00	NIST Webbook
rinpol	558.40	NIST Webbook
rinpol	559.40	NIST Webbook
rinpol	560.00	NIST Webbook
rinpol	559.00	NIST Webbook
rinpol	560.70	NIST Webbook
rinpol	559.00	NIST Webbook
rinpol	559.00	NIST Webbook
rinpol	557.39	NIST Webbook

rinpol	559.00		NIST Webbook
rinpol	558.00		NIST Webbook
rinpol	558.00		NIST Webbook
rinpol	564.00		NIST Webbook
tb	328.75 ± 0.30	K	NIST Webbook
tb	328.80	K	KDB
tb	328.88	K	Isobaric vapor-liquid equilibrium for four binary systems of thiophene
tb	328.88	K	Isobaric vapor-liquid equilibrium for systems containing sulfur compounds
tb	328.90	K	NIST Webbook
tb	328.76 ± 0.10	K	NIST Webbook
tb	328.83 ± 0.25	K	NIST Webbook
tb	328.75 ± 0.30	K	NIST Webbook
tb	328.77 ± 0.30	K	NIST Webbook
tb	328.77 ± 0.20	K	NIST Webbook
tb	329.40 ± 1.00	K	NIST Webbook
tb	329.40 ± 0.60	K	NIST Webbook
tb	329.40 ± 0.60	K	NIST Webbook
tb	328.95 ± 0.60	K	NIST Webbook
tb	328.95 ± 0.50	K	NIST Webbook
tb	329.15 ± 0.60	K	NIST Webbook
tb	328.76 ± 0.05	K	NIST Webbook
tb	329.40 ± 1.00	K	NIST Webbook
tb	328.85 ± 1.00	K	NIST Webbook
tb	329.65 ± 2.00	K	NIST Webbook
tb	328.79 ± 0.10	K	NIST Webbook
tb	328.35 ± 0.50	K	NIST Webbook
tc	497.70	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tc	501.00	K	KDB
tf	115.85 ± 0.06	K	NIST Webbook
tf	115.88 ± 0.05	K	NIST Webbook
tf	115.89 ± 0.03	K	NIST Webbook
tf	115.90 ± 0.40	K	NIST Webbook
tf	115.85 ± 0.06	K	NIST Webbook
tf	115.88 ± 0.04	K	NIST Webbook
tf	133.05 ± 0.20	K	NIST Webbook
tf	151.65 ± 2.00	K	NIST Webbook
tf	115.90	K	KDB
vc	0.343	m3/kmol	KDB
zc	0.2667870		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.07	J/mol×K	507.19	Joback Method
cpg	155.99	J/mol×K	361.86	Joback Method
cpg	165.99	J/mol×K	390.93	Joback Method
cpg	175.58	J/mol×K	419.99	Joback Method
cpg	184.79	J/mol×K	449.06	Joback Method
cpg	193.61	J/mol×K	478.12	Joback Method
cpg	145.57	J/mol×K	332.80	Joback Method
hvapt	27.41	kJ/mol	328.80	KDB
hvapt	30.50	kJ/mol	301.00	NIST Webbook
pvap	391.70	kPa	377.37	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K
pvap	158.10	kPa	343.06	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K
pvap	162.30	kPa	343.95	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K
pvap	171.30	kPa	345.83	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K
pvap	178.20	kPa	347.12	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K

pvap	186.40	kPa	348.71	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K
pvap	196.30	kPa	350.49	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K
pvap	208.60	kPa	352.78	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K
pvap	211.30	kPa	353.27	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K
pvap	216.30	kPa	354.06	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K
pvap	228.90	kPa	356.15	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K
pvap	244.90	kPa	358.73	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K

pvap	262.10	kPa	361.30	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K
pvap	273.70	kPa	362.89	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K
pvap	275.30	kPa	363.19	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K
pvap	284.90	kPa	364.38	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K
pvap	292.70	kPa	365.57	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K
pvap	303.80	kPa	366.96	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K
pvap	313.90	kPa	368.24	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K

pvap	319.70	kPa	369.04	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K
pvap	328.60	kPa	370.13	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K
pvap	153.70	kPa	341.87	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K
pvap	346.10	kPa	372.21	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K
pvap	351.50	kPa	372.90	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K
pvap	358.80	kPa	373.70	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K
pvap	366.70	kPa	374.59	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K

pvap	372.10	kPa	375.19	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K
pvap	377.40	kPa	375.78	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K
pvap	386.80	kPa	376.87	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K
pvap	336.40	kPa	371.12	Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K
rfi	1.38729		298.15	KDB
rhol	678.00	kg/m3	293.00	KDB
srf	0.02	N/m	298.20	KDB
tcondl	0.11	W/m×K	294.53	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	259.29	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.12	W/m×K	259.40	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.11	W/m×K	278.29	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.11	W/m×K	278.63	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.11	W/m×K	278.87	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.11	W/m×K	294.18	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.12	W/m×K	258.98	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.11	W/m×K	294.78	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.10	W/m×K	312.86	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.10	W/m×K	313.23	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.10	W/m×K	313.50	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	

tcondl	0.10	W/m×K	322.51	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.10	W/m×K	322.90	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.10	W/m×K	323.18	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.10	W/m×K	326.52	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.10	W/m×K	326.91	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	

tcondl	0.10	W/m×K	327.21	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	1.40939e+01
Coeff. B	-2.82259e+03
Coeff. C	-3.08790e+01
Temperature range (K), min.	235.32
Temperature range (K), max.	352.27

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.78292e+01
Coeff. B	-5.63780e+03
Coeff. C	-8.07579e+00
Coeff. D	6.84617e-06
Temperature range (K), min.	115.89
Temperature range (K), max.	500.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol210.mol
Isobaric vapor-liquid equilibrium for four binary systems of thiophene:	https://www.doi.org/10.1016/j.fluid.2011.11.020
Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons:	https://www.doi.org/10.1021/je034162x
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=210

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C563780&Units=SI
Isothermal Vapor-Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 348.06 K, 353.27 K, 363.19 K, and 372.90 K:	https://www.doi.org/10.1021/je101304x
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons:	https://www.doi.org/10.1021/je0341357
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Isobaric vapor-liquid equilibrium for systems containing sulfur compounds:	https://www.doi.org/10.1016/j.fluid.2013.05.019
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas 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
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
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility