1-Propene, 2-methyl-

Other names:	1,1-Dimethylethene
	1,1-Dimethylethylene
	2-METHYL PROPENE
	2-Methyl-1-propene
	2-Methylpropene
	2-Methylpropylene
	2-methylprop-1-ene
	ISOBUTYLENE
	Isobutene
	Isopropylidenemethylene
	Methylpropene
	Propene, 2-methyl-
	UN 1055
	iso-C4H8
	«gamma»-Butylene
	Â«gammaÂ»-Butylene
Inchi:	InChI=1S/C4H8/c1-4(2)3/h1H2,2-3H3
InchiKey:	VQTUBCCKSQIDNK-UHFFFAOYSA-N
Formula:	C4H8
SMILES:	C=C(C)C
Mol. weight [g/mol]:	56.11
CAS:	115-11-7

Physical Properties

Property code	Value	Unit	Source
af	0.1940		KDB
affp	802.10	kJ/mol	NIST Webbook
affp	802.30 ± 4.80	kJ/mol	NIST Webbook
affp	802.30 ± 4.80	kJ/mol	NIST Webbook
affp	805.00 ± 6.70	kJ/mol	NIST Webbook
aigt	738.15	K	KDB
ap	288.050	K	KDB
basg	776.30 ± 2.70	kJ/mol	NIST Webbook
basg	775.60	kJ/mol	NIST Webbook
basg	776.30 ± 2.70	kJ/mol	NIST Webbook
chg	-2699.50 ± 1.00	kJ/mol	NIST Webbook
chg	-2722.00	kJ/mol	NIST Webbook

dm	0.50	debye	KDB
fll	1.80	% in Air	KDB
flu	9.60	% in Air	KDB
fpo	197.04	K	KDB
gf	58.11	kJ/mol	KDB
hcg	2679.27	kJ/mol	KDB
hcn	2503.204	kJ/mol	KDB
hf	-16.91	kJ/mol	KDB
hf	-17.90 ± 1.10	kJ/mol	NIST Webbook
hfus	3.53	kJ/mol	Joback Method
hvap	20.60	kJ/mol	NIST Webbook
ie	9.24 ± 0.00	eV	NIST Webbook
ie	9.21	eV	NIST Webbook
ie	9.24 ± 0.02	eV	NIST Webbook
ie	9.23 ± 0.02	eV	NIST Webbook
ie	9.19	eV	NIST Webbook
ie	9.17	eV	NIST Webbook
ie	9.22 ± 0.02	eV	NIST Webbook
ie	9.24 ± 0.05	eV	NIST Webbook
ie	9.23	eV	NIST Webbook
ie	9.41	eV	NIST Webbook
ie	9.45	eV	NIST Webbook
ie	9.39	eV	NIST Webbook
ie	9.19	eV	NIST Webbook
log10ws	-2.33		Aqueous Solubility Prediction Method
log10ws	-2.33		Estimated Solubility Method
logp	1.582		Crippen Method
mcvol	62.920	ml/mol	McGowan Method
pc	4009.80	kPa	Thermodynamic properties of the butenes Part I. Experimental densities, vapor pressures, and critical points
pc	4000.00	kPa	KDB
pc	4000.00 ± 10.00	kPa	NIST Webbook
pc	4000.31 ± 10.13	kPa	NIST Webbook
rhoc	235.09 ± 0.56	kg/m3	NIST Webbook
rhoc	233.96 ± 2.81	kg/m3	NIST Webbook
rinpol	388.00		NIST Webbook
rinpol	383.00		NIST Webbook
rinpol	390.00		NIST Webbook
rinpol	390.00		NIST Webbook
rinpol	388.00		NIST Webbook
rinpol	387.00		NIST Webbook

rinpol	383.00		NIST Webbook
rinpol	390.00		NIST Webbook
rinpol	386.00		NIST Webbook
rinpol	370.00		NIST Webbook
rinpol	385.00		NIST Webbook
rinpol	400.00		NIST Webbook
rinpol	383.00		NIST Webbook
rinpol	384.00		NIST Webbook
rinpol	391.00		NIST Webbook
rinpol	392.00		NIST Webbook
rinpol	382.00		NIST Webbook
rinpol	390.00		NIST Webbook
rinpol	384.00		NIST Webbook
rinpol	383.00		NIST Webbook
rinpol	383.00		NIST Webbook
rinpol	383.00		NIST Webbook
rinpol	380.00		NIST Webbook
rinpol	390.00		NIST Webbook
rinpol	390.00		NIST Webbook
rinpol	390.00		NIST Webbook
rinpol	389.00		NIST Webbook
rinpol	394.00		NIST Webbook
rinpol	391.00		NIST Webbook
rinpol	384.00		NIST Webbook
ripol	427.00		NIST Webbook
ripol	438.00		NIST Webbook
sg	293.59	J/mol×K	NIST Webbook
sl	194.00	J/mol×K	NIST Webbook
tb	266.26 ± 0.55	K	NIST Webbook
tb	266.30	K	NIST Webbook
tb	268.15 ± 1.50	K	NIST Webbook
tb	267.15 ± 1.50	K	NIST Webbook
tb	268.65 ± 1.50	K	NIST Webbook
tb	266.40 ± 0.50	K	NIST Webbook
tb	266.26	K	NIST Webbook
tb	267.15 ± 1.00	K	NIST Webbook
tb	266.55 ± 0.70	K	NIST Webbook
tb	266.35 ± 0.50	K	NIST Webbook
tb	266.65 ± 2.00	K	NIST Webbook
tb	266.20	K	KDB
tb	266.55 ± 0.30	K	NIST Webbook
tb	266.22 ± 0.20	K	NIST Webbook
tb	267.15 ± 2.00	K	NIST Webbook
tb	267.15 ± 2.00	K	NIST Webbook

tb	266.55 ± 1.00	K	NIST Webbook
tb	266.45 ± 0.50	K	NIST Webbook
tb	267.15 ± 2.00	K	NIST Webbook
tb	266.85 ± 1.00	K	NIST Webbook
tb	266.20 ± 0.50	K	NIST Webbook
tb	267.15 ± 1.50	K	NIST Webbook
tb	266.35 ± 0.20	K	NIST Webbook
tb	266.55 ± 0.50	K	NIST Webbook
tb	266.55 ± 2.00	K	NIST Webbook
tb	267.15 ± 2.00	K	NIST Webbook
tb	269.15 ± 2.00	K	NIST Webbook
tb	267.15 ± 1.00	K	NIST Webbook
tb	267.15 ± 2.00	K	NIST Webbook
tc	417.90	K	KDB
tc	417.88 ± 0.10	K	NIST Webbook
tc	417.90 ± 0.10	K	NIST Webbook
tc	420.15 ± 2.00	K	NIST Webbook
tf	132.45 ± 0.30	K	NIST Webbook
tf	132.95	K	Aqueous Solubility Prediction Method
tf	132.38	K	NIST Webbook
tf	125.40 ± 0.50	K	NIST Webbook
tf	132.70	K	KDB
tt	132.40 ± 0.20	K	NIST Webbook
vc	0.239	m3/kmol	KDB
vc	0.239	m3/kmol	NIST Webbook
zc	0.2751370		KDB
zra	0.27		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	91.67 ± 0.46	J/mol×K	312.15	NIST Webbook
cpg	100.25 ± 0.50	J/mol×K	353.15	NIST Webbook
cpg	75.86 ± 0.38	J/mol×K	239.15	NIST Webbook
cpg	82.89 ± 0.41	J/mol×K	272.15	NIST Webbook
cpl	121.30	J/mol×K	266.26	NIST Webbook
cpl	121.42	J/mol×K	253.10	NIST Webbook
hfust	5.92	kJ/mol	132.40	NIST Webbook
hfust	5.92	kJ/mol	132.40	NIST Webbook
hfust	5.92	kJ/mol	132.40	NIST Webbook

hvapt	22.20	kJ/mol	350.50	NIST Webbook
hvapt	22.80	kJ/mol	244.50	NIST Webbook
hvapt	22.20	kJ/mol	343.00	NIST Webbook
hvapt	22.70	kJ/mol	289.50	NIST Webbook
hvapt	23.10	kJ/mol	245.50	NIST Webbook
hvapt	22.12	kJ/mol	266.30	KDB
hvapt	22.30	kJ/mol	394.50	NIST Webbook
pvap	608.84	kPa	323.14	Isothermal Vapor Liquid Equilibrium for Binary 2-Methylpropene - C1-C4 Alcohol-Systems
pvap	1110.00	kPa	348.15	Vapor liquid equilibria of the 1,1-difluoroethane (HFC-152a) + isobutene system
pvap	466.10	kPa	312.59	Vapour liquid equilibrium for the systems diethyl sulphide + 1-butene, +cis-2-butene, +2-methylpropane, +2-methylpropene, +n-butane, +trans-2-butene
pvap	467.10	kPa	312.59	Phase equilibrium measurements for systems containing propanenitrile with tert-butyl ethyl ether and C4-hydrocarbons
pvap	133.00	kPa	273.15	(Vapour + liquid) equilibria of the {1,1,1-trifluoroethane (HFC-143a) + isobutene} system
pvap	224.00	kPa	288.15	(Vapour + liquid) equilibria of the {1,1,1-trifluoroethane (HFC-143a) + isobutene} system
pvap	353.00	kPa	303.15	(Vapour + liquid) equilibria of the {1,1,1-trifluoroethane (HFC-143a) + isobutene} system

pvap	538.00	kPa	318.15	(Vapour + liquid) equilibria of the {1,1,1-trifluoroethane (HFC-143a) + isobutene} system
pvap	787.00	kPa	333.15	(Vapour + liquid) equilibria of the {1,1,1-trifluoroethane (HFC-143a) + isobutene} system
pvap	1110.00	kPa	348.15	(Vapour + liquid) equilibria of the {1,1,1-trifluoroethane (HFC-143a) + isobutene} system
pvap	605.14	kPa	322.79	Isothermal Vapor Liquid Equilibrium for Binary 2-Methylpropene - C1-C4 Alcohol-Systems
pvap	608.94	kPa	323.11	Isothermal Vapor Liquid Equilibrium for Binary 2-Methylpropene - C1-C4 Alcohol-Systems
pvap	787.00	kPa	333.15	Vapor liquid equilibria of the 1,1-difluoroethane (HFC-152a) + isobutene system
pvap	609.14	kPa	323.14	Isothermal Vapor Liquid Equilibrium for Binary 2-Methylpropene - C1-C4 Alcohol-Systems
pvap	611.04	kPa	323.15	Isothermal Vapor Liquid Equilibrium for Binary 2-Methylpropene - C1-C4 Alcohol-Systems
pvap	607.94	kPa	323.07	Vapor-Liquid Equilibrium for 1-Propanol + 1-Butene, + cis-2-Butene, + 2-Methyl-propene, + trans-2-Butene, + n-Butane, and + 2-Methyl-propane

pvap	1546.20	kPa	364.51	Vapor Liquid Equilibrium for Six Binary Systems of C4-Hydrocarbons + 2-Propanone
pvap	1546.00	kPa	364.49	Isothermal Vapor Liquid Equilibrium for 2-Methylpropene + Methanol, + 1-Propanol, + 2-Propanol, + 2-Butanol, and + 2-Methyl-2-propanol Binary Systems at 364.5 K
pvap	1546.60	kPa	364.51	Isothermal Vapor Liquid Equilibrium for 2-Methylpropene + Methanol, + 1-Propanol, + 2-Propanol, + 2-Butanol, and + 2-Methyl-2-propanol Binary Systems at 364.5 K
pvap	1546.50	kPa	364.51	Isothermal Vapor Liquid Equilibrium for 2-Methylpropene + Methanol, + 1-Propanol, + 2-Propanol, + 2-Butanol, and + 2-Methyl-2-propanol Binary Systems at 364.5 K
pvap	1546.30	kPa	364.52	Isothermal Vapor Liquid Equilibrium for 2-Methylpropene + Methanol, + 1-Propanol, + 2-Propanol, + 2-Butanol, and + 2-Methyl-2-propanol Binary Systems at 364.5 K
pvap	413.70	kPa	308.13	Vapor-Liquid Equilibrium for Thiophene + Butane, + trans-But-2-ene, + 2-Methylpropane, and + 2-Methylpropene

pvap	855.50	kPa	336.84	Vapor-Liquid Equilibrium for Thiophene + Butane, + trans-But-2-ene, + 2-Methylpropane, and + 2-Methylpropene
pvap	1154.30	kPa	350.43	Vapor-Liquid Equilibrium for Dimethyl Disulfide + Butane, + trans-But-2-ene, + 2-Methylpropane, + 2-Methylpropene, + Ethanol, and 2-Ethoxy-2-methylpropane
pvap	223.00	kPa	288.15	Vapor-Liquid Equilibria of the 1,1,1,2,3,3,3-Heptafluoropropane + Isobutene System
pvap	538.00	kPa	318.15	Vapor liquid equilibria of the 1,1-difluoroethane (HFC-152a) + isobutene system
pvap	536.00	kPa	318.15	Vapor-Liquid Equilibria of the 1,1,1,2,3,3,3-Heptafluoropropane + Isobutene System
pvap	785.00	kPa	333.15	Vapor-Liquid Equilibria of the 1,1,1,2,3,3,3-Heptafluoropropane + Isobutene System
pvap	1107.00	kPa	348.15	Vapor-Liquid Equilibria of the 1,1,1,2,3,3,3-Heptafluoropropane + Isobutene System
pvap	1515.00	kPa	363.15	Vapor-Liquid Equilibria of the 1,1,1,2,3,3,3-Heptafluoropropane + Isobutene System
pvap	542.10	kPa	318.35	Vapor-Liquid Equilibrium for Tetrahydrothiophene + n-Butane, + trans-2-Butene, + 2-Methylpropane, and + 2-Methylpropene

pvap	1054.90	kPa	346.14	Vapor-Liquid Equilibrium for Tetrahydrothiophene + n-Butane, + trans-2-Butene, + 2-Methylpropane, and + 2-Methylpropene
pvap	353.00	kPa	303.15	Vapor liquid equilibria of the 1,1-difluoroethane (HFC-152a) + isobutene system
pvap	224.00	kPa	288.15	Vapor liquid equilibria of the 1,1-difluoroethane (HFC-152a) + isobutene system
pvap	133.00	kPa	273.15	Vapor liquid equilibria of the 1,1-difluoroethane (HFC-152a) + isobutene system
pvap	465.30	kPa	312.60	Isothermal binary vapour liquid equilibrium for butanes and butenes with dimethylsulphide
pvap	538.15	kPa	318.40	Vapour liquid equilibrium for the ethyl ethanoate + 1-butene, +cis-2-butene, +trans-2-butene, +2-methylpropene, +n-butane and +2-methylpropane
pvap	352.00	kPa	303.15	Vapor-Liquid Equilibria of the 1,1,1,2,3,3,3-Heptafluoropropane + Isobutene System
rhol	594.00	kg/m3	293.00	KDB
sfust	44.71	J/mol×K	132.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40957e+01
Coeff. B	-2.26626e+03

Coeff. C	-2.70260e+01
Temperature range (K), min.	191.15
Temperature range (K), max.	285.02

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.75294e+01
Coeff. B	-4.53316e+03
Coeff. C	-8.37142e+00
Coeff. D	1.22482e-05
Temperature range (K), min.	132.81
Temperature range (K), max.	417.90

Sources

Vapour liquid equilibrium for the ethyl ethanoate + 1-butene, +cis-2-butene, +trans-2-butene, +2-methylpropene, +1,3-butadiene and +2-methylpropane:	https://www.doi.org/10.1016/j.fluid.2004.10.023
Henry's constants and infinite dilution activity coefficients of propane, propene, butane, isobutane, 1-butene, isobutene, trans-2-butene, and 1,3-butadiene in isobutanol and tert-butanol:	https://www.doi.org/10.1016/j.jct.2004.05.010
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Thermodynamic properties of the butenes Part I. Experimental densities, vapor pressures, and critical points:	https://www.doi.org/10.1016/j.fluid.2004.09.013
Vapor liquid equilibria of the 1,1-difluoroethane (HFC-152a) + isobutene system:	https://www.doi.org/10.1016/j.fluid.2008.07.007
Vapour liquid equilibrium for the systems diethyl sulphide + 1-butene, +cis-2-butene, +2-methylpropane, +2-methylpropene, +n-butane, +trans-2-butene:	https://www.doi.org/10.1016/j.fluid.2010.01.006
Vapor-Liquid Equilibrium for Tetrahydrothiophene + n-Butane, + trans-2-Butene, + 2-Methylpropane, and + 2-Methylpropene:	https://www.doi.org/10.1021/je800896m
Vapor-Liquid Equilibrium for Six Binary Systems of C4-Hydrocarbons + 2-Propanone:	https://www.doi.org/10.1021/je050403k
Henry's law constants and infinite dilution activity coefficients of propane, propene, butane, isobutane, 1-butene, isobutene, trans-2-butene and 1,3-butadiene in 2-methyl-1-butanol, 3-methyl-1-butanol and 2-methyl-2-butanol:	https://www.doi.org/10.1021/je049723e
Isothermal binary vapour liquid equilibrium for butanes and butenes with dimethyl sulphide:	https://www.doi.org/10.1016/j.fluid.2008.01.030
Vapor-Liquid Equilibrium for Dimethyl Disulfide + Butane, + trans-But-2-ene, + 2-Methylpropane, + 2-Methylpropene, + Ethanol, and 2-Ethoxy-2-methylpropane:	https://www.doi.org/10.1021/je200039y
Phase equilibrium measurements for systems containing propanenitrile with C4-hydrocarbons:	https://www.doi.org/10.1016/j.fluid.2010.09.023
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Vapor-Liquid Equilibrium for Thiophene + Butane, + trans-But-2-ene, + 2-Methylpropane, + 2-Methylpropene:	https://www.doi.org/10.1021/je101343m
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Henry's Law Constants and Infinite Dilution Activity Coefficients of Propane, Propene, Butane, 2-Methylpropane, 1-Butene, 2-Methylpropene, trans-2-Butene, cis-2-Butene, 1,3-Butadiene, Dimethyl Ether, Chloroethane, and 1,1-Difluoroethane in 2-Methylphenol, 3-Methylphenol, and 4-Methylphenol:	https://www.doi.org/10.1021/je0502647
	http://link.springer.com/article/10.1007/BF02311772
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2-methylpropane, trans-2-butene, and 2-methyl-2-propanol at 374.490K:	https://www.doi.org/10.1016/j.fluid.2006.06.024
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=189
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Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
(Vapour + liquid) equilibria of the {1,1,1-trifluoroethane (HFC-143a) + isobutene} system:	https://www.doi.org/10.1016/j.jct.2008.01.014

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Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Henry's Law Constants and Infinite Dilution Activity Coefficients of Propane, Propene, Butane, 2-Methylpropane, 1-Butene, [illegible]	https://www.doi.org/10.1021/je060395n
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Henry's Constants and Infinite Dilution Activity Coefficients of Propane, Propene, Butane, Isobutane, 1-Butene, Isobutene, trans-2-Butene and 1,3-Butadiene in 1-Butanol and 2-Butanol at (250 to 330) K:	https://www.doi.org/10.1021/je034265f
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C115117&Units=SI
KDB:	https://www.cheric.org/files/research/kdb/mol/mol189.mol
Isothermal Vapor Liquid Equilibrium for Binary 2-Methylpropene - C1-C4 Alcohol-Systems:	https://www.doi.org/10.1021/je034136z

Legend

af:	Acentric Factor
affp:	Proton affinity
aigt:	Autoignition Temperature
ap:	Aniline Point
basg:	Gas basicity
chg:	Standard gas enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
fll:	Lower Flammability Limit
flu:	Upper Flammability Limit
fpo:	Flash Point (Open Cup Method)
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
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
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
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
zc:	Critical Compressibility
zra:	Rackett Parameter