1-Butene, 3,3-dimethyl-

Other names:	(CH3)3CCH=CH2
	2,2-Dimethyl-3-butene
	3,3-Dimethyl-1-butene
	3,3-Dimethylbut-1-ene
	3,3-Dimethylbutene
	NEOHEXENE
	NSC 74119
	TERT-BUTYLETHENE
	TERT-HEXENE
	Trimethylvinylmethane
	tert-Butylethylene
Inchi:	InChI=1S/C6H12/c1-5-6(2,3)4/h5H,1H2,2-4H3
InchiKey:	PKXHXOTZMFCXSH-UHFFFAOYSA-N
Formula:	C6H12
SMILES:	C=CC(C)(C)C
Mol. weight [g/mol]:	84.16
CAS:	558-37-2

Physical Properties

Property code	Value	Unit	Source
af	0.1210		KDB
gf	98.22	kJ/mol	KDB
hcg	3988.65	kJ/mol	KDB
hcn	3724.555	kJ/mol	KDB
hf	-61.55	kJ/mol	KDB
hfus	2.60	kJ/mol	Joback Method
hvap	26.60	kJ/mol	NIST Webbook
hvap	26.60	kJ/mol	NIST Webbook
hvap	26.60	kJ/mol	NIST Webbook
hvap	27.40	kJ/mol	NIST Webbook
ie	9.62 ± 0.04	eV	NIST Webbook
ie	9.45 ± 0.01	eV	NIST Webbook
ie	9.45 ± 0.02	eV	NIST Webbook
ie	9.70	eV	NIST Webbook
ie	9.44	eV	NIST Webbook
log10ws	-1.95		Crippen Method
logp	2.219		Crippen Method

mcvol	91.100	ml/mol	McGowan Method
pc	3250.00	kPa	KDB
rinpol	510.00		NIST Webbook
rinpol	510.00		NIST Webbook
rinpol	507.40		NIST Webbook
rinpol	506.00		NIST Webbook
rinpol	513.00		NIST Webbook
rinpol	513.10		NIST Webbook
rinpol	512.00		NIST Webbook
rinpol	510.00		NIST Webbook
rinpol	509.00		NIST Webbook
rinpol	517.00		NIST Webbook
rinpol	507.40		NIST Webbook
rinpol	513.00		NIST Webbook
rinpol	517.00		NIST Webbook
rinpol	513.10		NIST Webbook
rinpol	515.00		NIST Webbook
rinpol	517.00		NIST Webbook
rinpol	515.00		NIST Webbook
rinpol	510.00		NIST Webbook
rinpol	509.00		NIST Webbook
rinpol	507.00		NIST Webbook
rinpol	506.00		NIST Webbook
rinpol	515.00		NIST Webbook
rinpol	507.00		NIST Webbook
rinpol	507.00		NIST Webbook
rinpol	509.00		NIST Webbook
rinpol	514.00		NIST Webbook
rinpol	505.00		NIST Webbook
rinpol	505.30		NIST Webbook
rinpol	513.90		NIST Webbook
rinpol	514.00		NIST Webbook
rinpol	505.00		NIST Webbook
sg	343.76	J/mol×K	NIST Webbook
sl	156.50	J/mol×K	NIST Webbook
tb	314.37 ± 0.20	K	NIST Webbook
tb	314.43 ± 0.10	K	NIST Webbook
tb	314.15 ± 1.50	K	NIST Webbook
tb	314.60 ± 0.50	K	NIST Webbook
tb	314.40 ± 3.00	K	NIST Webbook
tb	314.00 ± 4.00	K	NIST Webbook
tb	314.38 ± 0.20	K	NIST Webbook
tb	314.55 ± 0.40	K	NIST Webbook
tb	314.35 ± 0.50	K	NIST Webbook

tb	314.37 ± 0.20	K	NIST Webbook
tb	313.50 ± 0.50	K	NIST Webbook
tb	314.15 ± 0.30	K	NIST Webbook
tb	314.35 ± 1.00	K	NIST Webbook
tb	314.35 ± 0.50	K	NIST Webbook
tb	314.60 ± 0.50	K	NIST Webbook
tb	314.38 ± 0.05	K	NIST Webbook
tb	314.65 ± 2.00	K	NIST Webbook
tb	314.35 ± 0.50	K	NIST Webbook
tb	314.33 ± 0.20	K	NIST Webbook
tb	314.25 ± 0.50	K	NIST Webbook
tb	314.35 ± 0.50	K	NIST Webbook
tb	314.40	K	KDB
tb	314.40	K	NIST Webbook
tb	314.36 ± 0.20	K	NIST Webbook
tc	477.40	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tc	490.00	K	KDB
tf	158.08 ± 0.50	K	NIST Webbook
tf	157.62 ± 0.06	K	NIST Webbook
tf	157.92 ± 0.05	K	NIST Webbook
tf	157.88 ± 0.07	K	NIST Webbook
tf	158.00	K	KDB
tf	157.91 ± 0.40	K	NIST Webbook
tt	158.40 ± 0.20	K	NIST Webbook
vc	0.340	m3/kmol	KDB
zc	0.2712250		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.63	J/mol×K	508.46	Joback Method
cpg	178.54	J/mol×K	419.29	Joback Method
cpg	168.11	J/mol×K	389.57	Joback Method
cpg	157.12	J/mol×K	359.85	Joback Method
cpg	145.53	J/mol×K	330.13	Joback Method
cpg	197.78	J/mol×K	478.73	Joback Method
cpg	188.42	J/mol×K	449.01	Joback Method
cpl	188.28	J/mol×K	295.90	NIST Webbook
dvisc	0.0002699	Pa×s	330.13	Joback Method

dvisc	0.0005272	Pa×s	272.77	Joback Method
dvisc	0.0008290	Pa×s	244.09	Joback Method
dvisc	0.0014706	Pa×s	215.40	Joback Method
dvisc	0.0031112	Pa×s	186.72	Joback Method
dvisc	0.0003654	Pa×s	301.45	Joback Method
dvisc	0.0086393	Pa×s	158.04	Joback Method
hfust	1.09	kJ/mol	158.40	NIST Webbook
hvapt	25.65	kJ/mol	314.40	KDB
hvapt	28.60	kJ/mol	285.00	NIST Webbook
rfi	1.37313		298.15	KDB
rhol	653.00	kg/m3	293.00	KDB
srf	0.01	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39108e+01
Coeff. B	-2.56964e+03
Coeff. C	-3.78610e+01
Temperature range (K), min.	226.48
Temperature range (K), max.	336.68

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.15833e+01
Coeff. B	-5.85339e+03
Coeff. C	-1.03191e+01
Coeff. D	1.00976e-05
Temperature range (K), min.	157.95
Temperature range (K), max.	490.00

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol211.mol

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C558372&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons:	https://www.doi.org/10.1021/je0341357
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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=211
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
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
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
sg:	Molar entropy at standard conditions
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
zc:	Critical Compressibility