1-Pentene, 3-methyl-

Other names:	3-METHYL-1-PENTENE
	3-Methylpentene-1
	3-methylpent-1-ene
	C2H5CH(CH3)CH=CH2
	SEC-BUTYLETHENE
Inchi:	InChI=1S/C6H12/c1-4-6(3)5-2/h4,6H,1,5H2,2-3H3
InchiKey:	LDTAOIUHUHHCMU-UHFFFAOYSA-N
Formula:	C6H12
SMILES:	C=CC(C)CC
Mol. weight [g/mol]:	84.16
CAS:	760-20-3

Physical Properties

Property code	Value	Unit	Source
af	0.2620		KDB
gf	85.04	kJ/mol	Joback Method
hcg	3997.98	kJ/mol	KDB
hcn	3733.885	kJ/mol	KDB
hf	-47.02	kJ/mol	Joback Method
hfus	6.49	kJ/mol	Joback Method
hvap	28.60	kJ/mol	NIST Webbook
hvap	28.60	kJ/mol	NIST Webbook
hvap	28.60	kJ/mol	NIST Webbook
ie	9.44	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	3290.00	kPa	KDB
rinpol	551.80		NIST Webbook
rinpol	562.40		NIST Webbook
rinpol	563.00		NIST Webbook
rinpol	563.50		NIST Webbook
rinpol	558.00		NIST Webbook
rinpol	557.00		NIST Webbook
rinpol	561.00		NIST Webbook
rinpol	558.20		NIST Webbook

rinpol	558.80	NIST Webbook
rinpol	559.30	NIST Webbook
rinpol	559.90	NIST Webbook
rinpol	560.60	NIST Webbook
rinpol	561.20	NIST Webbook
rinpol	560.80	NIST Webbook
rinpol	560.50	NIST Webbook
rinpol	559.70	NIST Webbook
rinpol	559.20	NIST Webbook
rinpol	558.40	NIST Webbook
rinpol	557.80	NIST Webbook
rinpol	549.00	NIST Webbook
rinpol	562.00	NIST Webbook
rinpol	553.00	NIST Webbook
rinpol	551.50	NIST Webbook
rinpol	552.90	NIST Webbook
rinpol	554.00	NIST Webbook
rinpol	551.00	NIST Webbook
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rinpol	560.00	NIST Webbook
rinpol	548.00	NIST Webbook
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rinpol	558.00		NIST Webbook
rinpol	558.00		NIST Webbook
rinpol	551.80		NIST Webbook
rinpol	549.00		NIST Webbook
rinpol	549.70		NIST Webbook
rinpol	559.00		NIST Webbook
rinpol	557.60		NIST Webbook
rinpol	591.00		NIST Webbook
tb	327.33 ± 0.20	K	NIST Webbook
tb	326.95 ± 0.60	K	NIST Webbook
tb	326.95 ± 0.50	K	NIST Webbook
tb	327.35 ± 0.40	K	NIST Webbook
tb	327.30	K	KDB
tb	327.33 ± 0.40	K	NIST Webbook
tb	326.75 ± 0.50	K	NIST Webbook
tb	327.00	K	NIST Webbook
tb	327.40	K	NIST Webbook
tb	327.37 ± 0.20	K	NIST Webbook
tb	326.95 ± 0.60	K	NIST Webbook
tb	327.33 ± 0.30	K	NIST Webbook
tb	327.35 ± 0.50	K	NIST Webbook
tb	326.15 ± 2.00	K	NIST Webbook
tc	495.30	K	KDB
tf	118.60 ± 0.50	K	NIST Webbook

tf	120.00	K	KDB
tf	118.60 ± 1.00	K	NIST Webbook
vc	0.346	m3/kmol	KDB
zc	0.2768180		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	145.52	J/mol×K	332.92	Joback Method
cpg	155.75	J/mol×K	361.38	Joback Method
cpg	165.59	J/mol×K	389.85	Joback Method
cpg	175.03	J/mol×K	418.31	Joback Method
cpg	184.10	J/mol×K	446.78	Joback Method
cpg	192.81	J/mol×K	475.24	Joback Method
cpg	201.16	J/mol×K	503.71	Joback Method
dvisc	0.0022681	Pa×s	172.67	Joback Method
dvisc	0.0069474	Pa×s	140.62	Joback Method
dvisc	0.0010513	Pa×s	204.72	Joback Method
dvisc	0.0006001	Pa×s	236.77	Joback Method
dvisc	0.0003915	Pa×s	268.82	Joback Method
dvisc	0.0002798	Pa×s	300.87	Joback Method
dvisc	0.0002133	Pa×s	332.92	Joback Method
hvapt	26.90	kJ/mol	327.30	KDB
hvapt	30.00	kJ/mol	299.00	NIST Webbook
rfi	1.38133		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42678e+01
Coeff. B	-2.86795e+03
Coeff. C	-3.01180e+01
Temperature range (K), min.	235.26
Temperature range (K), max.	350.33

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.84660e+01
Coeff. B	-5.90299e+03
Coeff. C	-9.82952e+00
Coeff. D	1.03342e-05
Temperature range (K), min.	120.20
Temperature range (K), max.	495.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C760203&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=202
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=202
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas 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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility