2-Pentene, 3-methyl-, (E)-

Other names: (E)-3-methyl-2-pentene
(E)-3-methylpent-2-ene
(E)-CH3CH=C(CH3)C2H5
3-methyl-trans-2-pentene
trans-3-methyl-2-pentene
Inchi: InChI=1S/C6H12/c1-4-6(3)5-2/h4H,5H2,1-3H3/b6-4+
InchiKey: BEQGRRJLJLVQAQ-GQCTYLIASA-N
Formula: C6H12
SMILES: C/C=C(\C)CC
Mol. weight [g/mol]: 84.16
CAS: 616-12-6

Physical Properties

Property code	Value	Unit	Source
af	0.2070		KDB
gf	71.34	kJ/mol	KDB
hcg	3981.54	kJ/mol	KDB
hcn	3717.442	kJ/mol	KDB
hf	-63.51 ± 0.88	kJ/mol	NIST Webbook
hf	-63.14	kJ/mol	KDB
hfl	-94.93 ± 0.84	kJ/mol	NIST Webbook
hfus	10.19	kJ/mol	Joback Method
hvap	31.30	kJ/mol	NIST Webbook
hvap	30.00	kJ/mol	NIST Webbook
hvap	31.30	kJ/mol	NIST Webbook
hvap	32.10	kJ/mol	NIST Webbook
ie	8.63	eV	Cheméo Relay (1.0)
logp	2.363		Crippen Method
mcvol	91.100	ml/mol	McGowan Method
pc	3290.00	kPa	KDB
rinpol	615.42		NIST Webbook
rinpol	608.00		NIST Webbook
rinpol	620.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	625.00		NIST Webbook

rinpol	625.00	NIST Webbook
rinpol	625.00	NIST Webbook
rinpol	620.00	NIST Webbook
rinpol	620.80	NIST Webbook
rinpol	621.00	NIST Webbook
rinpol	621.20	NIST Webbook
rinpol	621.50	NIST Webbook
rinpol	621.70	NIST Webbook
rinpol	622.00	NIST Webbook
rinpol	622.50	NIST Webbook
rinpol	622.00	NIST Webbook
rinpol	621.20	NIST Webbook
rinpol	620.40	NIST Webbook
rinpol	619.60	NIST Webbook
rinpol	619.00	NIST Webbook
rinpol	623.00	NIST Webbook
rinpol	612.30	NIST Webbook
rinpol	612.80	NIST Webbook
rinpol	612.46	NIST Webbook
rinpol	613.00	NIST Webbook
rinpol	610.50	NIST Webbook
rinpol	613.00	NIST Webbook
rinpol	613.00	NIST Webbook
rinpol	612.00	NIST Webbook
rinpol	613.00	NIST Webbook
rinpol	613.00	NIST Webbook
rinpol	614.00	NIST Webbook
rinpol	614.00	NIST Webbook
rinpol	603.00	NIST Webbook
rinpol	612.00	NIST Webbook
rinpol	597.00	NIST Webbook
rinpol	622.20	NIST Webbook
rinpol	622.00	NIST Webbook
rinpol	620.80	NIST Webbook
rinpol	615.32	NIST Webbook
rinpol	620.00	NIST Webbook
rinpol	615.00	NIST Webbook
rinpol	620.00	NIST Webbook
rinpol	619.20	NIST Webbook
rinpol	619.70	NIST Webbook
rinpol	603.75	NIST Webbook
rinpol	612.50	NIST Webbook
rinpol	611.00	NIST Webbook
rinpol	603.00	NIST Webbook

rinpol	620.00		NIST Webbook
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rinpol	617.00		NIST Webbook
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rinpol	620.00		NIST Webbook
rinpol	619.00		NIST Webbook
rinpol	620.00		NIST Webbook
rinpol	620.00		NIST Webbook
rinpol	613.30		NIST Webbook
rinpol	613.10		NIST Webbook
rinpol	620.90		NIST Webbook
ripol	662.00		NIST Webbook
ripol	650.00		NIST Webbook
tb	343.59 ± 0.30	K	NIST Webbook
tb	343.79 ± 0.50	K	NIST Webbook
tb	341.05 ± 1.50	K	NIST Webbook
tb	343.60	K	KDB
tb	343.60	K	NIST Webbook
tb	343.59 ± 0.10	K	NIST Webbook
tb	343.50 ± 0.50	K	NIST Webbook
tb	343.75 ± 0.50	K	NIST Webbook
tb	343.20 ± 1.00	K	NIST Webbook
tb	340.15 ± 2.00	K	NIST Webbook

tb	343.65 ± 0.50	K	NIST Webbook
tb	343.65 ± 0.20	K	NIST Webbook
tc	521.00	K	KDB
tf	134.65 ± 0.20	K	NIST Webbook
tf	134.70	K	KDB
tf	134.69 ± 0.50	K	NIST Webbook
vc	0.350	m3/kmol	KDB
zc	0.2658210		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	145.07	J/mol×K	340.72	Joback Method
cpg	155.60	J/mol×K	370.05	Joback Method
cpg	165.66	J/mol×K	399.37	Joback Method
cpg	175.29	J/mol×K	428.70	Joback Method
cpg	184.49	J/mol×K	458.03	Joback Method
cpg	193.27	J/mol×K	487.36	Joback Method
cpg	201.67	J/mol×K	516.68	Joback Method
hvapt	29.29	kJ/mol	343.60	KDB
hvapt	32.80	kJ/mol	314.50	NIST Webbook
rfi	1.40166		298.15	KDB
rhol	698.00	kg/m3	293.00	KDB
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39511e+01
Coeff. B	-2.76043e+03
Coeff. C	-4.78120e+01
Temperature range (K), min.	249.84
Temperature range (K), max.	367.32

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.10543e+02
Coeff. B	-7.59988e+03
Coeff. C	-1.46143e+01
Coeff. D	1.31810e-05
Temperature range (K), min.	250.00
Temperature range (K), max.	521.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=206
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=206
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C616126&Units=SI
Measurements of activity coefficients at infinite dilution for organic solutes in two quaternary ammonium-based ionic liquids [DDA][ClO4] and [DDA][BF4]:	https://www.doi.org/10.1016/j.fluid.2018.11.011
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
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
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility