1-Butene, 2,3,3-trimethyl-

Other names:	(CH3)3CC(CH3)=CH2
	2,3,3-Trimethyl-1-butene
	2,3,3-trimethylbut-1-ene
	TRIPTENE
Inchi:	InChI=1S/C7H14/c1-6(2)7(3,4)5/h1H2,2-5H3
InchiKey:	AUYRUAVCWOAHQN-UHFFFAOYSA-N
Formula:	C7H14
SMILES:	C=C(C)C(C)(C)C
Mol. weight [g/mol]:	98.19
CAS:	594-56-9

Physical Properties

Property code	Value	Unit	Source
af	0.1920		KDB
ap	308.350	K	KDB
chl	-4637.70 ± 1.20	kJ/mol	NIST Webbook
gf	90.19	kJ/mol	Joback Method
hcg	4637.67	kJ/mol	KDB
hcn	4329.604	kJ/mol	KDB
hf	-86.54	kJ/mol	KDB
hfus	3.88	kJ/mol	Joback Method
hvap	34.30	kJ/mol	NIST Webbook
hvap	32.10	kJ/mol	NIST Webbook
ie	9.02 ± 0.01	eV	NIST Webbook
log10ws	-2.36		Crippen Method
logp	2.609		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	2890.00	kPa	KDB
rinpol	631.00		NIST Webbook
rinpol	634.00		NIST Webbook
rinpol	643.00		NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	621.00		NIST Webbook
rinpol	633.30		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	638.00		NIST Webbook

rinpol	640.00		NIST Webbook
rinpol	643.00		NIST Webbook
rinpol	639.10		NIST Webbook
rinpol	641.40		NIST Webbook
rinpol	628.60		NIST Webbook
rinpol	630.90		NIST Webbook
rinpol	634.00		NIST Webbook
rinpol	634.00		NIST Webbook
rinpol	632.00		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	633.00		NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	631.00		NIST Webbook
rinpol	633.00		NIST Webbook
rinpol	621.00		NIST Webbook
rinpol	631.65		NIST Webbook
rinpol	636.20		NIST Webbook
rinpol	627.00		NIST Webbook
rinpol	627.10		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	632.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	631.00		NIST Webbook
rinpol	637.00		NIST Webbook
rinpol	633.30		NIST Webbook
rinpol	636.00		NIST Webbook
rinpol	633.00		NIST Webbook
rinpol	632.00		NIST Webbook
rinpol	634.00		NIST Webbook
rinpol	631.65		NIST Webbook
rinpol	636.00		NIST Webbook
tb	351.00	K	KDB
tc	533.00	K	KDB
tf	163.15 ± 0.06	K	NIST Webbook
tf	153.25 ± 0.30	K	NIST Webbook
tf	161.25 ± 0.50	K	NIST Webbook
tf	161.30 ± 0.50	K	NIST Webbook
tf	163.30	K	KDB
tf	161.75 ± 0.10	K	NIST Webbook
vc	0.400	m3/kmol	KDB
zc	0.2608520		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.89	J/mol×K	352.89	Joback Method
cpg	194.04	J/mol×K	383.23	Joback Method
cpg	206.50	J/mol×K	413.58	Joback Method
cpg	218.32	J/mol×K	443.92	Joback Method
cpg	229.52	J/mol×K	474.26	Joback Method
cpg	240.13	J/mol×K	504.60	Joback Method
cpg	250.18	J/mol×K	534.95	Joback Method
hvapt	32.40	kJ/mol	320.50	NIST Webbook
hvapt	32.10	kJ/mol	319.50	NIST Webbook
rfi	1.40007		298.15	KDB
rhol	705.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40003e+01
Coeff. B	-2.92266e+03
Coeff. C	-3.94820e+01
Temperature range (K), min.	252.62
Temperature range (K), max.	375.85

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.69686e+01
Coeff. B	-6.31675e+03
Coeff. C	-9.43880e+00
Coeff. D	7.82230e-06
Temperature range (K), min.	163.30
Temperature range (K), max.	531.00

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol248.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C594569&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=248
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

Legend

af:	Acentric Factor
ap:	Aniline Point
chl:	Standard liquid enthalpy of combustion
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
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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

zc: Critical Compressibility