Butane, 2,2,3,3-tetramethyl-

Other names: (CH3)3CC(CH3)3
2,2,3,3-Tetramethylbutane
Ethane, hexamethyl-
HEXAMETHYLETHANE
TETRAMETHYLBUTANE
Inchi: InChI=1S/C8H18/c1-7(2,3)8(4,5)6/h1-6H3
InchiKey: OMMLUKLXGSRPHK-UHFFFAOYSA-N
Formula: C8H18
SMILES: CC(C)(C)C(C)(C)C
Mol. weight [g/mol]: 114.23
CAS: 594-82-1

Physical Properties

Property code	Value	Unit	Source
af	0.2510		KDB
chs	-5451.50 ± 1.10	kJ/mol	NIST Webbook
chs	-5451.90 ± 1.80	kJ/mol	NIST Webbook
gf	22.16	kJ/mol	Joback Method
hf	-226.20	kJ/mol	NIST Webbook
hf	-225.90 ± 1.90	kJ/mol	NIST Webbook
hfs	-268.80 ± 1.90	kJ/mol	NIST Webbook
hfs	-269.10 ± 1.20	kJ/mol	NIST Webbook
hfus	1.65	kJ/mol	Joback Method
hsub	42.90	kJ/mol	NIST Webbook
hsub	43.37 ± 0.21	kJ/mol	NIST Webbook
hsub	43.40 ± 0.20	kJ/mol	NIST Webbook
hsub	42.90 ± 0.90	kJ/mol	NIST Webbook
hvap	42.91	kJ/mol	NIST Webbook
hvap	42.94	kJ/mol	NIST Webbook
ie	9.80	eV	NIST Webbook
ie	10.20 ± 0.05	eV	NIST Webbook
ie	10.37	eV	NIST Webbook
ie	9.80	eV	NIST Webbook
ie	9.79	eV	NIST Webbook
log10ws	-2.69		Crippen Method
logp	3.079		Crippen Method
mcvol	123.580	ml/mol	McGowan Method

pc	2870.00	kPa	KDB
rinpol	720.00		NIST Webbook
rinpol	731.00		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	736.00		NIST Webbook
rinpol	733.28		NIST Webbook
rinpol	736.21		NIST Webbook
rinpol	739.23		NIST Webbook
rinpol	727.21		NIST Webbook
rinpol	730.14		NIST Webbook
rinpol	723.90		NIST Webbook
rinpol	722.00		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	728.00		NIST Webbook
rinpol	720.00		NIST Webbook
rinpol	723.70		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	720.00		NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	721.00		NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	731.00		NIST Webbook
rinpol	723.00		NIST Webbook
rinpol	728.00		NIST Webbook
rinpol	731.00		NIST Webbook
rinpol	729.00		NIST Webbook
rinpol	720.00		NIST Webbook
rinpol	716.00		NIST Webbook
rinpol	710.35		NIST Webbook
rinpol	712.98		NIST Webbook
rinpol	714.69		NIST Webbook
rinpol	712.25		NIST Webbook
rinpol	730.20		NIST Webbook
rinpol	716.46		NIST Webbook
rinpol	726.10		NIST Webbook
rinpol	719.00		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	676.00		NIST Webbook
rinpol	729.00		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	714.80		NIST Webbook

rinpol	733.00		NIST Webbook
rinpol	726.00		NIST Webbook
sg	389.30 ± 1.30	J/mol×K	NIST Webbook
ss	256.90	J/mol×K	NIST Webbook
ss	273.76	J/mol×K	NIST Webbook
tb	379.60	K	KDB
tc	567.80	K	KDB
tf	373.80	K	KDB
tt	373.97 ± 0.07	K	NIST Webbook
vc	0.461	m3/kmol	KDB
zc	0.2802530		KDB
zra	0.27		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.16	J/mol×K	500.01	Joback Method
cpg	307.15	J/mol×K	531.02	Joback Method
cpg	233.87	J/mol×K	375.98	Joback Method
cpg	250.27	J/mol×K	406.99	Joback Method
cpg	265.77	J/mol×K	438.00	Joback Method
cpg	280.38	J/mol×K	469.01	Joback Method
cpg	319.38	J/mol×K	562.03	Joback Method
cps	239.62	J/mol×K	301.60	NIST Webbook
cps	232.20	J/mol×K	295.40	NIST Webbook
dvisc	0.0007345	Pa×s	312.24	Joback Method
dvisc	0.0004645	Pa×s	344.11	Joback Method
dvisc	0.0003175	Pa×s	375.98	Joback Method
dvisc	0.0223115	Pa×s	184.76	Joback Method
dvisc	0.0065211	Pa×s	216.63	Joback Method
dvisc	0.0026130	Pa×s	248.50	Joback Method
dvisc	0.0012890	Pa×s	280.37	Joback Method
hfust	7.54	kJ/mol	373.90	NIST Webbook
hfust	7.54	kJ/mol	373.90	NIST Webbook
hfust	2.00	kJ/mol	152.50	NIST Webbook
hsubt	43.60	kJ/mol	331.50	NIST Webbook
hsubt	56.20	kJ/mol	271.00	NIST Webbook
hvapt	333.00	kJ/mol	383.50	NIST Webbook
hvapt	31.42	kJ/mol	379.60	KDB
sfust	20.16	J/mol×K	373.90	NIST Webbook
sfust	13.11	J/mol×K	152.50	NIST Webbook

srf	0.02	N/m	298.20	KDB

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	379.70	K	102.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.31777e+01
Coeff. B	-2.51762e+03
Coeff. C	-8.53050e+01
Temperature range (K), min.	280.62
Temperature range (K), max.	405.36

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.32058e+02
Coeff. B	-9.96316e+03
Coeff. C	-1.72776e+01
Coeff. D	9.39147e-06
Temperature range (K), min.	270.00
Temperature range (K), max.	567.80

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol63.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C594821&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=63
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
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation 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
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
srf:	Surface Tension
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter