Neopentane

Other names:	1,1,1-Trimethylethane
	2,2-Dimethylpropane
	Dimethylpropane
	Neo-C5H12
	Propane, 2,2-dimethyl-
	Tetramethylcarbon
	Tetramethylmethane
	UN 2044
	tert-Pentane
Inchi:	InChI=1S/C5H12/c1-5(2,3)4/h1-4H3
InchiKey:	CRSOQBOWXPBRES-UHFFFAOYSA-N
Formula:	C5H12
SMILES:	CC(C)(C)C
Mol. weight [g/mol]:	72.15
CAS:	463-82-1

Physical Properties

Property code	Value	Unit	Source
chg	-3514.10 ± 0.96	kJ/mol	NIST Webbook
chl	-3494.40 ± 1.00	kJ/mol	NIST Webbook
chl	-3492.40 ± 0.59	kJ/mol	NIST Webbook
gf	-5.94	kJ/mol	Joback Method
hf	-167.90 ± 0.63	kJ/mol	NIST Webbook
hf	-166.00 ± 1.00	kJ/mol	NIST Webbook
hf	-168.50 ± 1.00	kJ/mol	NIST Webbook
hfl	-190.30 ± 0.63	kJ/mol	NIST Webbook
hfl	-188.20 ± 1.00	kJ/mol	NIST Webbook
hfus	1.29	kJ/mol	Joback Method
hvap	21.85	kJ/mol	NIST Webbook
hvap	22.40 ± 0.59	kJ/mol	NIST Webbook
hvap	22.39	kJ/mol	NIST Webbook
hvap	21.80	kJ/mol	NIST Webbook
ie	10.35	eV	NIST Webbook
ie	11.30	eV	NIST Webbook
ie	10.30 ± 0.08	eV	NIST Webbook
ie	10.90 ± 0.10	eV	NIST Webbook
ie	10.90	eV	NIST Webbook

ie	10.21 ± 0.04	eV	NIST Webbook
ie	10.30 ± 0.10	eV	NIST Webbook
ie	10.40	eV	NIST Webbook
ie	11.30	eV	NIST Webbook
log10ws	-1.67		Crippen Method
logp	2.052		Crippen Method
mcvol	81.310	ml/mol	McGowan Method
pc	3200.00 ± 10.00	kPa	NIST Webbook
pc	3196.30 ± 10.13	kPa	NIST Webbook
pc	3199.00 ± 20.27	kPa	NIST Webbook
rhoc	235.21 ± 0.72	kg/m3	NIST Webbook
rhoc	231.89 ± 2.16	kg/m3	NIST Webbook
rinpol	412.00		NIST Webbook
rinpol	412.00		NIST Webbook
rinpol	415.30		NIST Webbook
rinpol	413.00		NIST Webbook
rinpol	414.00		NIST Webbook
rinpol	410.60		NIST Webbook
rinpol	409.00		NIST Webbook
rinpol	409.00		NIST Webbook
rinpol	415.00		NIST Webbook
rinpol	413.00		NIST Webbook
rinpol	413.00		NIST Webbook
rinpol	412.30		NIST Webbook
rinpol	412.00		NIST Webbook
rinpol	407.60		NIST Webbook
rinpol	415.00		NIST Webbook
rinpol	413.00		NIST Webbook
rinpol	412.50		NIST Webbook
rinpol	413.00		NIST Webbook
rinpol	408.80		NIST Webbook
rinpol	409.80		NIST Webbook
rinpol	410.60		NIST Webbook
rinpol	411.30		NIST Webbook
rinpol	411.80		NIST Webbook
rinpol	412.10		NIST Webbook
rinpol	409.00		NIST Webbook
rinpol	407.60		NIST Webbook
rinpol	412.00		NIST Webbook
rinpol	413.00		NIST Webbook
rinpol	411.00		NIST Webbook
rinpol	413.00		NIST Webbook
rinpol	413.00		NIST Webbook
rinpol	413.00		NIST Webbook

rinpol	411.00		NIST Webbook
rinpol	412.00		NIST Webbook
rinpol	413.00		NIST Webbook
rinpol	412.00		NIST Webbook
rinpol	415.30		NIST Webbook
rinpol	413.00		NIST Webbook
rinpol	412.00		NIST Webbook
rinpol	414.00		NIST Webbook
rinpol	414.00		NIST Webbook
rinpol	408.40		NIST Webbook
sl	218.80	J/mol×K	NIST Webbook
sl	216.81	J/mol×K	NIST Webbook
tb	282.65 ± 2.00	K	NIST Webbook
tb	282.65 ± 1.00	K	NIST Webbook
tb	283.00 ± 2.00	K	NIST Webbook
tb	282.15 ± 1.00	K	NIST Webbook
tb	282.75 ± 0.50	K	NIST Webbook
tb	282.60 ± 0.50	K	NIST Webbook
tb	282.56 ± 0.20	K	NIST Webbook
tb	282.15 ± 3.00	K	NIST Webbook
tb	282.65 ± 2.00	K	NIST Webbook
tb	282.65 ± 0.10	K	NIST Webbook
tb	282.15 ± 2.00	K	NIST Webbook
tb	282.15 ± 2.00	K	NIST Webbook
tb	282.70	K	NIST Webbook
tb	282.70	K	NIST Webbook
tb	282.65 ± 0.30	K	NIST Webbook
tb	282.75 ± 0.30	K	NIST Webbook
tb	282.65 ± 0.30	K	NIST Webbook
tc	433.80	K	NIST Webbook
tc	433.80 ± 0.20	K	NIST Webbook
tc	433.75 ± 0.10	K	NIST Webbook
tc	433.75 ± 0.20	K	NIST Webbook
tc	433.80 ± 0.10	K	NIST Webbook
tf	256.60 ± 0.03	K	NIST Webbook
tf	253.00 ± 5.00	K	NIST Webbook
tf	252.65 ± 1.00	K	NIST Webbook
tf	254.15 ± 2.00	K	NIST Webbook
tf	256.55 ± 0.05	K	NIST Webbook
tf	253.80 ± 0.60	K	NIST Webbook
tf	256.57 ± 0.04	K	NIST Webbook
tf	253.65 ± 0.50	K	NIST Webbook
tt	256.53 ± 0.02	K	NIST Webbook
tt	256.77 ± 0.03	K	NIST Webbook

tt	256.76 ± 0.02	K	NIST Webbook
vc	0.304 ± 0.004	m3/kmol	NIST Webbook
vc	0.307	m3/kmol	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.38 ± 0.39	J/mol×K	523.15	NIST Webbook
cpg	129.58 ± 0.26	J/mol×K	323.15	NIST Webbook
cpg	120.82 ± 0.25	J/mol×K	298.15	NIST Webbook
cpg	155.46 ± 0.31	J/mol×K	398.15	NIST Webbook
cpg	163.52 ± 0.32	J/mol×K	423.15	NIST Webbook
cpg	171.46 ± 0.34	J/mol×K	448.15	NIST Webbook
cpg	178.95 ± 0.36	J/mol×K	473.15	NIST Webbook
cpg	186.42 ± 0.37	J/mol×K	498.15	NIST Webbook
cpg	147.06 ± 0.29	J/mol×K	373.15	NIST Webbook
cpg	138.41 ± 0.28	J/mol×K	348.15	NIST Webbook
cpl	153.09	J/mol×K	259.93	NIST Webbook
cpl	163.89	J/mol×K	278.92	NIST Webbook
dvisc	0.0034432	Pa×s	175.54	Joback Method
dvisc	0.0015845	Pa×s	202.54	Joback Method
dvisc	0.0008752	Pa×s	229.55	Joback Method
dvisc	0.0005478	Pa×s	256.56	Joback Method
dvisc	0.0003749	Pa×s	283.56	Joback Method
dvisc	0.0099225	Pa×s	148.53	Joback Method
dvisc	0.0002740	Pa×s	310.57	Joback Method
hfust	2.58	kJ/mol	140.00	NIST Webbook
hfust	3.26	kJ/mol	256.50	NIST Webbook
hfust	3.26	kJ/mol	256.50	NIST Webbook
hsubt	23.90	kJ/mol	210.00	NIST Webbook
hsubt	28.20	kJ/mol	239.50	NIST Webbook
hvapt	22.80 ± 0.10	kJ/mol	283.00	NIST Webbook
hvapt	22.20	kJ/mol	290.00	NIST Webbook
hvapt	19.50	kJ/mol	330.00	NIST Webbook
hvapt	16.20	kJ/mol	370.00	NIST Webbook
hvapt	11.10	kJ/mol	410.00	NIST Webbook
hvapt	22.80	kJ/mol	388.00	NIST Webbook
hvapt	23.10	kJ/mol	407.50	NIST Webbook
hvapt	23.10	kJ/mol	348.50	NIST Webbook
hvapt	24.00	kJ/mol	290.50	NIST Webbook
hvapt	24.30	kJ/mol	275.00	NIST Webbook

hvapt	22.75	kJ/mol	282.61	NIST Webbook
hvapt	22.74	kJ/mol	282.70	NIST Webbook
sfust	12.69	J/mol×K	256.50	NIST Webbook
sfust	18.41	J/mol×K	140.00	NIST Webbook
svapt	80.50	J/mol×K	282.61	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.55175e+01
Coeff. B	-4.67668e+03
Coeff. C	-8.00342e+00
Coeff. D	1.02687e-05
Temperature range (K), min.	256.58
Temperature range (K), max.	433.78

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/files/research/kdb/mol/mol34.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C463821&Units=SI

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=34

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Bubble Point Measurements of Neopentane + Ethane Mixtures: https://www.doi.org/10.1021/acs.jced.8b01106

Legend

chg: Standard gas enthalpy of combustion

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

cpl: Liquid phase heat capacity

dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
rhoc:	Critical density
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
svapt:	Entropy of vaporization at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume