Pentane, 2,3,3-trimethyl-

Other names: 2,3,3-Trimethylpentane
C2H5C(CH3)2CH(CH3)2
Inchi: InChI=1S/C8H18/c1-6-8(4,5)7(2)3/h7H,6H2,1-5H3
InchiKey: OKVWYBALHQFVFP-UHFFFAOYSA-N
Formula: C8H18
SMILES: CCC(C)(C)C(C)C
Mol. weight [g/mol]: 114.23
CAS: 560-21-4

Physical Properties

Property code	Value	Unit	Source
af	0.2900		KDB
ap	340.150	K	KDB
chl	-5467.00 ± 1.30	kJ/mol	NIST Webbook
gf	18.92	kJ/mol	KDB
hcg	5466.98	kJ/mol	KDB
hcn	5070.841	kJ/mol	KDB
hf	-216.40 ± 1.40	kJ/mol	NIST Webbook
hf	-216.60	kJ/mol	KDB
hfl	-253.70 ± 1.40	kJ/mol	NIST Webbook
hfus	5.54	kJ/mol	Joback Method
hvap	37.20 ± 0.10	kJ/mol	NIST Webbook
hvap	36.90	kJ/mol	NIST Webbook
hvap	37.60 ± 0.10	kJ/mol	NIST Webbook
hvap	37.21	kJ/mol	NIST Webbook
hvap	37.70 ± 0.10	kJ/mol	NIST Webbook
hvap	37.20	kJ/mol	NIST Webbook
hvap	36.90 ± 0.10	kJ/mol	NIST Webbook
hvap	37.33	kJ/mol	NIST Webbook
hvap	36.90 ± 0.10	kJ/mol	NIST Webbook
log10ws	-2.69		Crippen Method
logp	3.079		Crippen Method
mcvol	123.580	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
pc	2820.00	kPa	KDB
pc	2820.00 ± 40.00	kPa	NIST Webbook
pc	2820.20 ± 40.53	kPa	NIST Webbook

rhoc	251.30 ± 4.57	kg/m3	NIST Webbook
rhoc	251.30 ± 4.57	kg/m3	NIST Webbook
rinpol	753.00		NIST Webbook
rinpol	764.00		NIST Webbook
rinpol	761.00		NIST Webbook
rinpol	757.00		NIST Webbook
rinpol	764.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	767.00		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	720.60		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	757.00		NIST Webbook
rinpol	755.00		NIST Webbook
rinpol	759.60		NIST Webbook
rinpol	768.00		NIST Webbook
rinpol	755.40		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	762.00		NIST Webbook
rinpol	763.09		NIST Webbook
rinpol	759.00		NIST Webbook
rinpol	770.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	759.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	767.00		NIST Webbook
rinpol	759.00		NIST Webbook
rinpol	749.00		NIST Webbook
rinpol	755.00		NIST Webbook
rinpol	762.00		NIST Webbook
rinpol	761.00		NIST Webbook
rinpol	757.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	749.00		NIST Webbook
rinpol	720.60		NIST Webbook
rinpol	759.00		NIST Webbook

rinpol	767.00		NIST Webbook
rinpol	761.00		NIST Webbook
rinpol	764.80		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	761.40		NIST Webbook
rinpol	761.30		NIST Webbook
rinpol	761.40		NIST Webbook
rinpol	761.40		NIST Webbook
rinpol	761.40		NIST Webbook
rinpol	757.00		NIST Webbook
rinpol	758.50		NIST Webbook
rinpol	762.75		NIST Webbook
rinpol	756.90		NIST Webbook
rinpol	757.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	761.00		NIST Webbook
rinpol	759.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	764.53		NIST Webbook
rinpol	767.27		NIST Webbook
rinpol	769.65		NIST Webbook
rinpol	759.95		NIST Webbook
rinpol	762.11		NIST Webbook
rinpol	755.00		NIST Webbook
rinpol	757.00		NIST Webbook
rinpol	755.00		NIST Webbook
rinpol	757.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	759.00		NIST Webbook
rinpol	761.00		NIST Webbook
rinpol	757.00		NIST Webbook
tb	386.00 ± 2.00	K	NIST Webbook
tb	387.90	K	NIST Webbook
tb	387.90	K	NIST Webbook
tb	387.94 ± 0.10	K	NIST Webbook
tb	387.91 ± 0.20	K	NIST Webbook
tb	387.40 ± 2.00	K	NIST Webbook
tb	387.40 ± 0.40	K	NIST Webbook
tb	387.85 ± 0.30	K	NIST Webbook
tb	390.45 ± 0.50	K	NIST Webbook
tb	387.65 ± 0.30	K	NIST Webbook
tb	387.75 ± 0.30	K	NIST Webbook
tb	387.85 ± 0.30	K	NIST Webbook

tb	387.91 ± 0.10	K	NIST Webbook
tb	387.85 ± 0.50	K	NIST Webbook
tb	387.91 ± 0.02	K	NIST Webbook
tb	388.05 ± 0.20	K	NIST Webbook
tb	383.95 ± 0.60	K	NIST Webbook
tb	388.05 ± 0.20	K	NIST Webbook
tb	387.91 ± 0.05	K	NIST Webbook
tb	387.85 ± 0.30	K	NIST Webbook
tb	387.80 ± 0.50	K	NIST Webbook
tb	387.90	K	KDB
tc	573.49 ± 0.40	K	NIST Webbook
tc	573.50	K	KDB
tc	573.50 ± 0.50	K	NIST Webbook
tf	170.75 ± 0.50	K	NIST Webbook
tf	172.18 ± 0.04	K	NIST Webbook
tf	172.19 ± 0.02	K	NIST Webbook
tf	170.75 ± 1.00	K	NIST Webbook
tf	171.55 ± 0.15	K	NIST Webbook
tf	170.15 ± 1.00	K	NIST Webbook
tf	170.75 ± 0.50	K	NIST Webbook
tf	171.49 ± 0.02	K	NIST Webbook
tf	171.80 ± 0.15	K	NIST Webbook
tf	172.45 ± 0.10	K	NIST Webbook
tf	172.11 ± 0.12	K	NIST Webbook
tf	171.45 ± 0.10	K	NIST Webbook
tf	172.17 ± 0.05	K	NIST Webbook
tf	171.73 ± 0.20	K	NIST Webbook
tf	172.22	K	KDB
vc	0.455	m3/kmol	NIST Webbook
vc	0.455	m3/kmol	KDB
zc	0.2690860		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.27	J/mol×K	557.09	Joback Method
cpg	248.05	J/mol×K	408.49	Joback Method
cpg	262.39	J/mol×K	438.21	Joback Method
cpg	276.06	J/mol×K	467.93	Joback Method
cpg	289.08	J/mol×K	497.65	Joback Method
cpg	301.48	J/mol×K	527.37	Joback Method

cpg	233.00	J/mol×K	378.77	Joback Method
cpl	245.56	J/mol×K	298.15	NIST Webbook
dvisc	0.0003870	Pa×s	343.53	Joback Method
dvisc	0.0006049	Pa×s	308.29	Joback Method
dvisc	0.0010608	Pa×s	273.06	Joback Method
dvisc	0.0021975	Pa×s	237.82	Joback Method
dvisc	0.0058649	Pa×s	202.58	Joback Method
dvisc	0.0002691	Pa×s	378.77	Joback Method
dvisc	0.0236666	Pa×s	167.34	Joback Method
hvapt	34.10 ± 0.10	kJ/mol	358.00	NIST Webbook
hvapt	33.50 ± 0.10	kJ/mol	368.00	NIST Webbook
hvapt	36.90 ± 0.10	kJ/mol	308.00	NIST Webbook
hvapt	36.50 ± 0.10	kJ/mol	315.00	NIST Webbook
hvapt	34.80 ± 0.10	kJ/mol	348.00	NIST Webbook
hvapt	35.50 ± 0.10	kJ/mol	330.00	NIST Webbook
hvapt	35.10 ± 0.10	kJ/mol	338.00	NIST Webbook
hvapt	34.40 ± 0.10	kJ/mol	348.00	NIST Webbook
hvapt	33.90 ± 0.10	kJ/mol	358.00	NIST Webbook
hvapt	33.30 ± 0.10	kJ/mol	368.00	NIST Webbook
hvapt	36.10	kJ/mol	345.00	NIST Webbook
hvapt	36.40	kJ/mol	349.00	NIST Webbook
hvapt	32.34	kJ/mol	387.90	KDB
hvapt	32.12	kJ/mol	387.90	NIST Webbook
hvapt	37.10 ± 0.10	kJ/mol	308.00	NIST Webbook
hvapt	35.10 ± 0.10	kJ/mol	338.00	NIST Webbook
hvapt	35.50 ± 0.10	kJ/mol	330.00	NIST Webbook
hvapt	36.00 ± 0.10	kJ/mol	323.00	NIST Webbook
hvapt	36.60 ± 0.10	kJ/mol	315.00	NIST Webbook
hvapt	36.00 ± 0.10	kJ/mol	323.00	NIST Webbook
rfi	1.40522		298.15	KDB
rhol	726.00	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	1.41778e+01
Coeff. B	-3.32462e+03
Coeff. C	-4.01370e+01

Temperature range (K), min.	279.49
Temperature range (K), max.	415.11

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.59740e+01
Coeff. B	-6.89717e+03
Coeff. C	-9.14884e+00
Coeff. D	6.39547e-06
Temperature range (K), min.	172.22
Temperature range (K), max.	573.50

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C560214&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=61

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/files/research/kdb/mol/mol61.mol

Legend

af: Acentric Factor

ap: Aniline Point

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

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-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