Pentane, 3-ethyl-3-methyl-

Other names:	3-ETHYL-3-METHYLPENTANE
	3-Methyl-3-ethylpentane
Inchi:	InChI=1S/C8H18/c1-5-8(4,6-2)7-3/h5-7H2,1-4H3
InchiKey:	GIEZWIDCIFCQPS-UHFFFAOYSA-N
Formula:	C8H18
SMILES:	CCC(C)(CC)CC
Mol. weight [g/mol]:	114.23
CAS:	1067-08-9

Physical Properties

Property code	Value	Unit	Source
af	0.3030		KDB
ap	339.050	K	KDB
chl	-5467.70 ± 1.10	kJ/mol	NIST Webbook
gf	19.93	kJ/mol	KDB
hcg	5467.65	kJ/mol	KDB
hcn	5071.510	kJ/mol	KDB
hf	-215.00 ± 1.30	kJ/mol	NIST Webbook
hf	-215.10	kJ/mol	KDB
hfl	-253.00 ± 1.30	kJ/mol	NIST Webbook
hfus	9.06	kJ/mol	Joback Method
hvap	38.00 ± 0.10	kJ/mol	NIST Webbook
hvap	38.00	kJ/mol	NIST Webbook
hvap	38.05	kJ/mol	NIST Webbook
hvap	37.98	kJ/mol	NIST Webbook
log10ws	-2.93		Crippen Method
logp	3.223		Crippen Method
mcvol	123.580	ml/mol	McGowan Method
pc	2810.00	kPa	KDB
pc	2807.30 ± 40.53	kPa	NIST Webbook
pc	2810.00 ± 40.00	kPa	NIST Webbook
rhoc	251.30 ± 4.57	kg/m3	NIST Webbook
rhoc	251.30 ± 4.57	kg/m3	NIST Webbook
rinpol	781.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	772.20		NIST Webbook
rinpol	769.00		NIST Webbook

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rinpol	769.00	NIST Webbook
rinpol	780.00	NIST Webbook
rinpol	780.00	NIST Webbook
rinpol	778.60	NIST Webbook
rinpol	776.00	NIST Webbook
rinpol	774.00	NIST Webbook
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rinpol	769.00	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	777.00	NIST Webbook
rinpol	771.20	NIST Webbook
rinpol	770.00	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	778.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	778.00	NIST Webbook
rinpol	764.00	NIST Webbook
rinpol	766.50	NIST Webbook
rinpol	768.40	NIST Webbook
rinpol	765.42	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	763.06	NIST Webbook
rinpol	765.47	NIST Webbook
rinpol	770.20	NIST Webbook
rinpol	764.38	NIST Webbook
rinpol	766.76	NIST Webbook
rinpol	768.22	NIST Webbook
rinpol	764.00	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	783.00	NIST Webbook
rinpol	778.00	NIST Webbook
rinpol	773.00	NIST Webbook
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rinpol	781.00		NIST Webbook
rinpol	764.00		NIST Webbook
rinpol	768.40		NIST Webbook
rinpol	766.94		NIST Webbook
rinpol	768.40		NIST Webbook
rinpol	776.90		NIST Webbook
rinpol	773.80		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	769.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	766.94		NIST Webbook
tb	391.55 ± 0.60	K	NIST Webbook
tb	391.41 ± 0.05	K	NIST Webbook
tb	391.40 ± 0.02	K	NIST Webbook
tb	391.55 ± 0.20	K	NIST Webbook
tb	391.50 ± 0.20	K	NIST Webbook
tb	391.42	K	KDB
tb	391.40	K	NIST Webbook
tb	391.40	K	NIST Webbook
tb	391.41 ± 0.20	K	NIST Webbook
tb	391.53 ± 0.20	K	NIST Webbook
tb	391.60 ± 0.30	K	NIST Webbook
tb	391.20 ± 0.30	K	NIST Webbook
tb	391.43 ± 0.20	K	NIST Webbook
tb	391.95 ± 0.30	K	NIST Webbook
tb	391.18 ± 0.30	K	NIST Webbook
tb	391.43 ± 0.15	K	NIST Webbook
tb	391.43 ± 0.30	K	NIST Webbook
tb	391.65 ± 0.30	K	NIST Webbook
tc	576.50 ± 0.50	K	NIST Webbook
tc	576.50	K	NIST Webbook
tc	576.51 ± 0.40	K	NIST Webbook
tc	576.50	K	KDB
tf	182.20	K	KDB
vc	0.455	m3/kmol	NIST Webbook
vc	0.455	m3/kmol	KDB
zc	0.2667360		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.27	J/mol×K	403.30	NIST Webbook
cpg	275.73	J/mol×K	462.60	NIST Webbook
cpg	303.76	J/mol×K	521.70	NIST Webbook
dvisc	0.0009261	Pa×s	280.77	Joback Method
dvisc	0.0005696	Pa×s	313.59	Joback Method
dvisc	0.0003841	Pa×s	346.40	Joback Method
dvisc	0.0002773	Pa×s	379.21	Joback Method
dvisc	0.0038192	Pa×s	215.15	Joback Method
dvisc	0.0017124	Pa×s	247.96	Joback Method
dvisc	0.0113690	Pa×s	182.34	Joback Method
hvapt	40.20	kJ/mol	320.00	NIST Webbook
hvapt	36.90	kJ/mol	352.50	NIST Webbook
hvapt	32.79	kJ/mol	391.40	KDB
hvapt	32.78	kJ/mol	391.40	NIST Webbook
rfi	1.40549		298.15	KDB
rhol	727.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42156e+01
Coeff. B	-3.35442e+03
Coeff. C	-4.19010e+01
Temperature range (K), min.	282.74
Temperature range (K), max.	418.63

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.90694e+01
Coeff. B	-7.10610e+03
Coeff. C	-9.60229e+00

Coeff. D	6.71857e-06
Temperature range (K), min.	182.28
Temperature range (K), max.	576.50

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1067089&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=58
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/mol58.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
ap:	Aniline Point
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhoc:	Critical density
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