Pentane, 3-ethyl-2-methyl-

Other names:	2-Methyl-3-ethylpentane
	3-ETHYL-2-METHYLPENTANE
Inchi:	InChI=1S/C8H18/c1-5-8(6-2)7(3)4/h7-8H,5-6H2,1-4H3
InchiKey:	DUPUVYJQZSLSJB-UHFFFAOYSA-N
Formula:	C8H18
SMILES:	CCC(CC)C(C)C
Mol. weight [g/mol]:	114.23
CAS:	609-26-7

Physical Properties

Property code	Value	Unit	Source
af	0.3300		KDB
ap	340.350	K	KDB
chl	-5471.00 ± 1.40	kJ/mol	NIST Webbook
gf	21.27	kJ/mol	KDB
hcg	5470.91	kJ/mol	KDB
hcn	5074.774	kJ/mol	KDB
hf	-211.30	kJ/mol	KDB
hf	-211.20 ± 1.30	kJ/mol	NIST Webbook
hfl	-249.70 ± 1.30	kJ/mol	NIST Webbook
hfus	9.43	kJ/mol	Joback Method
hvap	38.56	kJ/mol	NIST Webbook
hvap	38.50	kJ/mol	NIST Webbook
hvap	38.52	kJ/mol	NIST Webbook
hvap	38.50 ± 0.10	kJ/mol	NIST Webbook
log10ws	-2.69		Crippen Method
logp	3.079		Crippen Method
mcvol	123.580	ml/mol	McGowan Method
pc	2700.40 ± 40.53	kPa	NIST Webbook
pc	2700.00	kPa	KDB
pc	2700.00 ± 40.00	kPa	NIST Webbook
rhoc	258.16 ± 4.57	kg/m3	NIST Webbook
rhoc	258.16 ± 4.57	kg/m3	NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	755.00		NIST Webbook
rinpol	759.00		NIST Webbook
rinpol	760.00		NIST Webbook

rinpol	762.00	NIST Webbook
rinpol	763.00	NIST Webbook
rinpol	759.00	NIST Webbook
rinpol	762.00	NIST Webbook
rinpol	762.00	NIST Webbook
rinpol	756.00	NIST Webbook
rinpol	764.00	NIST Webbook
rinpol	767.00	NIST Webbook
rinpol	764.00	NIST Webbook
rinpol	761.00	NIST Webbook
rinpol	760.00	NIST Webbook
rinpol	755.00	NIST Webbook
rinpol	762.00	NIST Webbook
rinpol	762.00	NIST Webbook
rinpol	763.00	NIST Webbook
rinpol	762.75	NIST Webbook
rinpol	758.00	NIST Webbook
rinpol	760.00	NIST Webbook
rinpol	755.00	NIST Webbook
rinpol	758.00	NIST Webbook
rinpol	757.28	NIST Webbook
rinpol	765.00	NIST Webbook
rinpol	764.00	NIST Webbook
rinpol	755.00	NIST Webbook
rinpol	759.00	NIST Webbook
rinpol	762.00	NIST Webbook
rinpol	743.00	NIST Webbook
rinpol	755.00	NIST Webbook
rinpol	765.50	NIST Webbook
rinpol	758.00	NIST Webbook
rinpol	763.00	NIST Webbook
rinpol	759.00	NIST Webbook
rinpol	762.00	NIST Webbook
rinpol	765.00	NIST Webbook
rinpol	760.30	NIST Webbook
rinpol	762.75	NIST Webbook
rinpol	760.20	NIST Webbook
rinpol	761.50	NIST Webbook
rinpol	762.70	NIST Webbook
rinpol	763.80	NIST Webbook
rinpol	758.00	NIST Webbook
rinpol	759.00	NIST Webbook
rinpol	760.00	NIST Webbook
rinpol	762.00	NIST Webbook

rinpol	763.00		NIST Webbook
rinpol	762.40		NIST Webbook
rinpol	763.20		NIST Webbook
rinpol	763.30		NIST Webbook
rinpol	761.10		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	764.00		NIST Webbook
rinpol	762.00		NIST Webbook
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rinpol	758.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	762.00		NIST Webbook
rinpol	764.00		NIST Webbook
rinpol	755.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	759.00		NIST Webbook
rinpol	762.40		NIST Webbook
rinpol	755.95		NIST Webbook
rinpol	760.40		NIST Webbook
rinpol	759.70		NIST Webbook
rinpol	760.00		NIST Webbook
tb	388.81	K	KDB
tb	388.80	K	NIST Webbook
tb	388.80 ± 0.20	K	NIST Webbook
tb	387.15 ± 1.50	K	NIST Webbook
tb	388.85 ± 0.40	K	NIST Webbook

tb	388.80 ± 0.05	K	NIST Webbook
tb	388.85 ± 0.20	K	NIST Webbook
tb	388.85 ± 0.10	K	NIST Webbook
tb	388.80 ± 0.02	K	NIST Webbook
tb	388.70 ± 0.30	K	NIST Webbook
tb	388.80 ± 0.05	K	NIST Webbook
tb	388.90 ± 0.15	K	NIST Webbook
tb	388.65 ± 0.30	K	NIST Webbook
tb	388.55 ± 0.20	K	NIST Webbook
tb	388.70 ± 0.10	K	NIST Webbook
tb	388.80	K	NIST Webbook
tc	567.10	K	KDB
tc	567.10 ± 0.50	K	NIST Webbook
tc	567.00	K	NIST Webbook
tc	567.02 ± 0.40	K	NIST Webbook
tf	157.97 ± 0.20	K	NIST Webbook
tf	158.65 ± 0.50	K	NIST Webbook
tf	158.15 ± 0.20	K	NIST Webbook
tf	158.14 ± 0.05	K	NIST Webbook
tf	158.14 ± 0.06	K	NIST Webbook
tf	158.10 ± 0.02	K	NIST Webbook
tf	158.20	K	KDB
tf	157.97 ± 0.20	K	NIST Webbook
tf	158.21 ± 0.10	K	NIST Webbook
tf	157.97 ± 0.20	K	NIST Webbook
vc	0.442	m3/kmol	KDB
vc	0.442	m3/kmol	NIST Webbook
zc	0.2530990		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.57	J/mol×K	522.20	NIST Webbook
cpg	243.09	J/mol×K	399.70	NIST Webbook
cpg	272.80	J/mol×K	461.90	NIST Webbook
dvisc	0.0231912	Pa×s	149.92	Joback Method
dvisc	0.0004905	Pa×s	304.35	Joback Method
dvisc	0.0003218	Pa×s	342.95	Joback Method
dvisc	0.0002299	Pa×s	381.56	Joback Method
dvisc	0.0008449	Pa×s	265.74	Joback Method
dvisc	0.0017511	Pa×s	227.13	Joback Method

dvisc	0.0048914	Pa×s	188.53	Joback Method
hvapt	37.40	kJ/mol	350.50	NIST Webbook
hvapt	32.93	kJ/mol	388.80	NIST Webbook
rfi	1.40167		298.15	KDB
rhol	719.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41006e+01
Coeff. B	-3.19130e+03
Coeff. C	-5.22440e+01
Temperature range (K), min.	283.28
Temperature range (K), max.	415.34

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.38476e+01
Coeff. B	-7.34958e+03
Coeff. C	-1.02987e+01
Coeff. D	7.18885e-06
Temperature range (K), min.	250.00
Temperature range (K), max.	567.00

Sources

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol57.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C609267&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=57

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

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

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