

Pentane, 3-ethyl-

Other names:	3-Ethylpentane
Inchi:	InChI=1S/C7H16/c1-4-7(5-2)6-3/h7H,4-6H2,1-3H3
InchiKey:	AORMDLNPRGXHHL-UHFFFAOYSA-N
Formula:	C7H16
SMILES:	CCC(CC)CC
Mol. weight [g/mol]:	100.20
CAS:	617-78-7

Physical Properties

Property code	Value	Unit	Source
af	0.3100		KDB
ap	338.850	K	KDB
chl	-4814.00 ± 1.30	kJ/mol	NIST Webbook
chl	-4816.30 ± 1.10	kJ/mol	NIST Webbook
dm	0.00	debye	KDB
gf	11.00	kJ/mol	KDB
hcg	4816.33	kJ/mol	KDB
hcn	4464.203	kJ/mol	KDB
hf	-189.80	kJ/mol	KDB
hf	-191.40	kJ/mol	NIST Webbook
hf	-189.70 ± 1.20	kJ/mol	NIST Webbook
hfl	-226.70 ± 1.30	kJ/mol	NIST Webbook
hfl	-225.00 ± 1.20	kJ/mol	NIST Webbook
hfus	10.36	kJ/mol	Joback Method
hvap	35.32	kJ/mol	NIST Webbook
hvap	35.22	kJ/mol	NIST Webbook
hvap	35.20 ± 0.10	kJ/mol	NIST Webbook
hvap	35.10 ± 0.10	kJ/mol	NIST Webbook
hvap	35.20	kJ/mol	NIST Webbook
log10ws	-2.51		Crippen Method
logp	2.833		Crippen Method
mcvol	109.490	ml/mol	McGowan Method
pc	2890.00	kPa	KDB
pc	2890.00 ± 40.00	kPa	NIST Webbook
pc	2890.80 ± 40.53	kPa	NIST Webbook
pc	2897.90 ± 50.66	kPa	NIST Webbook
rhoc	241.49 ± 5.01	kg/m3	NIST Webbook

rhoc	241.49 ± 4.01	kg/m3	NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	687.00		NIST Webbook
rinpol	687.00		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	688.00		NIST Webbook
rinpol	683.00		NIST Webbook
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rinpol	682.00		NIST Webbook
rinpol	685.47		NIST Webbook
rinpol	684.98		NIST Webbook
rinpol	684.11		NIST Webbook
rinpol	685.24		NIST Webbook
rinpol	684.72		NIST Webbook
rinpol	683.88		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	685.00		NIST Webbook
rinpol	687.00		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	682.00		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	687.00		NIST Webbook
rinpol	682.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	682.20		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	682.17		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	688.00		NIST Webbook
rinpol	687.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	686.00		NIST Webbook

rinpol	683.00	NIST Webbook
rinpol	684.70	NIST Webbook
rinpol	682.20	NIST Webbook
rinpol	685.24	NIST Webbook
rinpol	687.00	NIST Webbook
rinpol	683.00	NIST Webbook
rinpol	687.30	NIST Webbook
rinpol	685.00	NIST Webbook
rinpol	687.00	NIST Webbook
rinpol	687.40	NIST Webbook
rinpol	687.40	NIST Webbook
rinpol	687.40	NIST Webbook
rinpol	687.90	NIST Webbook
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rinpol	687.50	NIST Webbook
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rinpol	685.50	NIST Webbook
rinpol	686.10	NIST Webbook
rinpol	686.60	NIST Webbook
rinpol	687.20	NIST Webbook
rinpol	687.00	NIST Webbook
rinpol	687.40	NIST Webbook
rinpol	686.00	NIST Webbook
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rinpol	679.00	NIST Webbook
rinpol	686.20	NIST Webbook
rinpol	686.40	NIST Webbook
rinpol	686.00	NIST Webbook
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rinpol	687.00	NIST Webbook
rinpol	683.50	NIST Webbook
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rinpol	682.00		NIST Webbook
rinpol	685.00		NIST Webbook
rinpol	685.90		NIST Webbook
rinpol	684.70		NIST Webbook
rinpol	679.79		NIST Webbook
rinpol	680.52		NIST Webbook
rinpol	687.00		NIST Webbook
sg	411.50	J/mol×K	NIST Webbook
sl	312.10	J/mol×K	NIST Webbook
sl	314.55	J/mol×K	NIST Webbook
tb	366.65 ± 0.50	K	NIST Webbook
tb	366.60	K	KDB
tb	366.70	K	NIST Webbook

tb	366.45 ± 0.50	K	NIST Webbook
tb	366.60	K	NIST Webbook
tb	366.40 ± 1.50	K	NIST Webbook
tb	366.63 ± 0.30	K	NIST Webbook
tb	366.60 ± 0.20	K	NIST Webbook
tb	366.47 ± 0.30	K	NIST Webbook
tb	366.62 ± 0.07	K	NIST Webbook
tb	366.45 ± 0.50	K	NIST Webbook
tb	366.45 ± 0.50	K	NIST Webbook
tb	366.52 ± 0.30	K	NIST Webbook
tb	366.62 ± 0.03	K	NIST Webbook
tb	366.61 ± 0.07	K	NIST Webbook
tb	366.52 ± 0.20	K	NIST Webbook
tb	366.60 ± 0.20	K	NIST Webbook
tb	366.70 ± 0.20	K	NIST Webbook
tb	366.62 ± 0.07	K	NIST Webbook
tb	366.70 ± 0.20	K	NIST Webbook
tb	366.60 ± 0.20	K	NIST Webbook
tb	366.70 ± 0.15	K	NIST Webbook
tb	366.62 ± 0.20	K	NIST Webbook
tb	366.57 ± 0.20	K	NIST Webbook
tb	366.40 ± 0.50	K	NIST Webbook
tc	540.75 ± 0.50	K	NIST Webbook
tc	540.60 ± 0.40	K	NIST Webbook
tc	540.60	K	KDB
tc	540.57 ± 0.40	K	NIST Webbook
tf	154.35 ± 0.30	K	NIST Webbook
tf	154.55 ± 0.01	K	NIST Webbook
tf	154.50 ± 0.06	K	NIST Webbook
tf	154.35 ± 0.50	K	NIST Webbook
tf	154.54 ± 0.02	K	NIST Webbook
tf	154.53 ± 0.03	K	NIST Webbook
tf	154.39 ± 0.30	K	NIST Webbook
tf	154.50	K	KDB
tf	154.25 ± 0.20	K	NIST Webbook
tt	154.59 ± 0.03	K	NIST Webbook
tt	154.58 ± 0.03	K	NIST Webbook
tt	154.58 ± 0.06	K	NIST Webbook
tt	154.58 ± 0.08	K	NIST Webbook
tt	154.58 ± 0.02	K	NIST Webbook
tt	154.59 ± 0.02	K	NIST Webbook
tt	154.30 ± 0.20	K	NIST Webbook
vc	0.416	m3/kmol	KDB
vc	0.416	m3/kmol	NIST Webbook

zc	0.2674720	KDB
zra	0.27	KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.02	J/mol×K	359.12	Joback Method
cpg	206.19	J/mol×K	387.02	Joback Method
cpg	217.92	J/mol×K	414.93	Joback Method
cpg	229.23	J/mol×K	442.83	Joback Method
cpg	240.13	J/mol×K	470.73	Joback Method
cpg	250.62	J/mol×K	498.63	Joback Method
cpg	260.72	J/mol×K	526.54	Joback Method
cpl	217.60	J/mol×K	294.80	NIST Webbook
cpl	219.58	J/mol×K	298.15	NIST Webbook
dvisc	0.0030264	Pa×s	187.90	Joback Method
dvisc	0.0003156	Pa×s	324.88	Joback Method
dvisc	0.0002348	Pa×s	359.12	Joback Method
dvisc	0.0004548	Pa×s	290.63	Joback Method
dvisc	0.0007226	Pa×s	256.38	Joback Method
dvisc	0.0099972	Pa×s	153.65	Joback Method
dvisc	0.0013243	Pa×s	222.14	Joback Method
hfust	9.46	kJ/mol	154.30	NIST Webbook
hfust	9.55	kJ/mol	154.58	NIST Webbook
hfust	9.55	kJ/mol	154.60	NIST Webbook
hfust	9.55	kJ/mol	154.60	NIST Webbook
hvapt	32.70 ± 0.10	kJ/mol	338.00	NIST Webbook
hvapt	34.50 ± 0.10	kJ/mol	308.00	NIST Webbook
hvapt	31.12	kJ/mol	366.60	NIST Webbook
hvapt	30.96	kJ/mol	366.60	KDB
hvapt	34.10 ± 0.10	kJ/mol	315.00	NIST Webbook
hvapt	35.20	kJ/mol	329.50	NIST Webbook
hvapt	33.70 ± 0.10	kJ/mol	232.00	NIST Webbook
hvapt	33.30 ± 0.10	kJ/mol	330.00	NIST Webbook
hvapt	35.00	kJ/mol	330.50	NIST Webbook
hvapt	32.20 ± 0.10	kJ/mol	348.00	NIST Webbook
hvapt	34.40	kJ/mol	349.50	NIST Webbook
rfi	1.39084		298.15	KDB
rhoI	698.00	kg/m3	293.00	KDB
sfust	61.77	J/mol×K	154.58	NIST Webbook
sfust	61.31	J/mol×K	154.30	NIST Webbook

srf	0.02	N/m	298.20	KDB	
tcondl	0.11	W/m×K	313.96	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)	
tcondl	0.11	W/m×K	296.78	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)	
tcondl	0.11	W/m×K	314.27	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)	
tcondl	0.11	W/m×K	314.58	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)	
tcondl	0.11	W/m×K	296.62	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)	
tcondl	0.11	W/m×K	296.33	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)	
tcondl	0.12	W/m×K	278.19	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)	

tcondl	0.12	W/m×K	277.89	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)
tcondl	0.13	W/m×K	257.83	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)
tcondl	0.13	W/m×K	257.54	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)
tcondl	0.13	W/m×K	257.28	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)
tcondl	0.10	W/m×K	331.22	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)
tcondl	0.10	W/m×K	331.29	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)
tcondl	0.10	W/m×K	331.56	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)

tcondl	0.12	W/m×K	277.62	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)
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Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.43548e+01
Coeff. B	-3.22861e+03
Coeff. C	-3.50210e+01
Temperature range (K), min.	264.53
Temperature range (K), max.	392.04

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	6.25346e+01
Coeff. B	-6.12547e+03
Coeff. C	-7.08145e+00
Coeff. D	4.46212e-06
Temperature range (K), min.	154.55
Temperature range (K), max.	540.64

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.thermo.com/files/research/kdb/mol/mol41.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8): NIST Webbook	https://www.doi.org/10.1021/je020125e http://webbook.nist.gov/cgi/cbook.cgi?ID=C617787&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
ap:	Aniline Point
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
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
hfust:	Enthalpy of fusion at a given temperature
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
rho:	Liquid Density
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility

zra:

Rackett Parameter

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