Pentane, 3,3-diethyl-

Other names:	3,3-Diethylpentane
	TETRAETHYLMETHANE
Inchi:	InChI=1S/C9H20/c1-5-9(6-2,7-3)8-4/h5-8H2,1-4H3
InchiKey:	BGXXXYLRPIRDHJ-UHFFFAOYSA-N
Formula:	C9H20
SMILES:	CCC(CC)(CC)CC
Mol. weight [g/mol]:	128.26
CAS:	1067-20-5

Physical Properties

Property code	Value	Unit	Source
af	0.3380		KDB
ap	338.150	K	KDB
chl	-6124.50 ± 1.60	kJ/mol	NIST Webbook
dm	0.00	debye	KDB
gf	35.09	kJ/mol	KDB
hcg	6124.50	kJ/mol	KDB
hcn	5684.383	kJ/mol	KDB
hf	-232.10	kJ/mol	KDB
hfus	11.65	kJ/mol	Joback Method
hvap	42.60 ± 0.30	kJ/mol	NIST Webbook
hvap	43.60	kJ/mol	NIST Webbook
hvap	42.03	kJ/mol	NIST Webbook
hvap	42.60 ± 0.30	kJ/mol	NIST Webbook
log10ws	-3.35		Crippen Method
logp	3.613		Crippen Method
mcvol	137.670	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
pc	2670.00	kPa	KDB
rinpol	882.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	880.62		NIST Webbook
rinpol	874.00		NIST Webbook

rinpol	875.20		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	880.62		NIST Webbook
rinpol	885.80		NIST Webbook
rinpol	880.20		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	877.10		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	877.60		NIST Webbook
rinpol	886.40		NIST Webbook
rinpol	875.60		NIST Webbook
rinpol	875.30		NIST Webbook
rinpol	882.40		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	871.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	877.50		NIST Webbook
rinpol	890.00		NIST Webbook
rinpol	886.90		NIST Webbook
sg	436.52	J/mol×K	NIST Webbook
sl	333.40	J/mol×K	NIST Webbook
tb	419.30 ± 0.20	K	NIST Webbook
tb	419.40	K	NIST Webbook
tb	412.35 ± 0.60	K	NIST Webbook
tb	419.35 ± 0.30	K	NIST Webbook
tb	419.55 ± 0.30	K	NIST Webbook
tb	418.90 ± 0.40	K	NIST Webbook
tb	419.55 ± 0.60	K	NIST Webbook
tb	419.31 ± 0.03	K	NIST Webbook
tb	419.35 ± 0.30	K	NIST Webbook
tb	419.32 ± 0.30	K	NIST Webbook
tb	419.32 ± 0.25	K	NIST Webbook
tb	418.83 ± 0.20	K	NIST Webbook
tb	419.40	K	NIST Webbook
tb	419.30	K	KDB
tc	610.00	K	KDB
tf	242.05 ± 0.60	K	NIST Webbook
tf	238.75 ± 0.30	K	NIST Webbook
tf	232.15 ± 4.00	K	NIST Webbook
tf	240.04 ± 0.03	K	NIST Webbook
tf	239.90 ± 0.20	K	NIST Webbook

tf	239.90 ± 0.30	K	NIST Webbook
tf	240.04 ± 0.01	K	NIST Webbook
tf	242.05 ± 0.30	K	NIST Webbook
tf	239.90 ± 0.30	K	NIST Webbook
tf	241.55 ± 0.50	K	NIST Webbook
tf	240.03 ± 0.15	K	NIST Webbook
tf	242.01 ± 0.20	K	NIST Webbook
tf	240.13 ± 0.10	K	NIST Webbook
tf	241.55 ± 0.40	K	NIST Webbook
tf	240.10	K	KDB
tt	240.10 ± 0.03	K	NIST Webbook
tt	240.13 ± 0.20	K	NIST Webbook
tt	240.11 ± 0.04	K	NIST Webbook
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.99	J/mol×K	402.09	Joback Method
cpg	289.63	J/mol×K	431.00	Joback Method
cpg	304.56	J/mol×K	459.91	Joback Method
cpg	318.82	J/mol×K	488.82	Joback Method
cpg	332.42	J/mol×K	517.74	Joback Method
cpg	345.39	J/mol×K	546.65	Joback Method
cpg	357.75	J/mol×K	575.56	Joback Method
cpl	278.20	J/mol×K	298.15	NIST Webbook
cpl	260.90	J/mol×K	260.00	NIST Webbook
cpl	278.80	J/mol×K	298.15	NIST Webbook
dvisc	0.0002652	Pa×s	402.09	Joback Method
dvisc	0.0003685	Pa×s	367.34	Joback Method
dvisc	0.0005485	Pa×s	332.60	Joback Method
dvisc	0.0008957	Pa×s	297.85	Joback Method
dvisc	0.0016651	Pa×s	263.10	Joback Method
dvisc	0.0037384	Pa×s	228.36	Joback Method
dvisc	0.0112198	Pa×s	193.61	Joback Method
hfust	0.48	kJ/mol	208.30	NIST Webbook
hfust	10.09	kJ/mol	240.10	NIST Webbook
hfust	0.81	kJ/mol	210.40	NIST Webbook
hfust	10.09	kJ/mol	240.10	NIST Webbook
hvapt	35.98	kJ/mol	419.30	KDB
hvapt	39.80	kJ/mol	380.50	NIST Webbook

hvapt	34.61	kJ/mol	419.40	NIST Webbook
rfi	1.41837		298.15	KDB
rhol	752.00	kg/m3	293.00	KDB
sfust	42.02	J/mol×K	240.10	NIST Webbook
sfust	3.85	J/mol×K	210.40	NIST Webbook
sfust	2.32	J/mol×K	208.30	NIST Webbook
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59178e+01
Coeff. B	-4.12066e+03
Coeff. C	-4.46790e+01
Temperature range (K), min.	308.31
Temperature range (K), max.	433.19

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.85614e+01
Coeff. B	-7.57215e+03
Coeff. C	-9.42583e+00
Coeff. D	5.85657e-06
Temperature range (K), min.	240.12
Temperature range (K), max.	610.05

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol90.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1067205&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=90

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

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
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
nfpaf:	NFPA Fire Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	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
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume