

Hexane, 2,2,5-trimethyl-

Other names:	2,2,5-Trimethylhexane
Inchi:	InChI=1S/C9H20/c1-8(2)6-7-9(3,4)5/h8H,6-7H2,1-5H3
InchiKey:	HHOSMYBYIHNXNO-UHFFFAOYSA-N
Formula:	C9H20
SMILES:	CC(C)CCC(C)(C)C
Mol. weight [g/mol]:	128.26
CAS:	3522-94-9

Physical Properties

Property code	Value	Unit	Source
af	0.3570		KDB
ap	355.850	K	KDB
chl	-6106.55 ± 0.84	kJ/mol	NIST Webbook
gf	13.44	kJ/mol	KDB
hcg	6106.55	kJ/mol	KDB
hcn	5666.434	kJ/mol	KDB
hf	-254.20	kJ/mol	KDB
hf	-253.10	kJ/mol	NIST Webbook
hfl	-293.30 ± 1.00	kJ/mol	NIST Webbook
hfus	8.13	kJ/mol	Joback Method
hvap	40.21	kJ/mol	NIST Webbook
hvap	40.20	kJ/mol	NIST Webbook
hvap	40.17	kJ/mol	NIST Webbook
hvap	40.20	kJ/mol	NIST Webbook
log10ws	-5.05		Estimated Solubility Method
log10ws	-5.05		Aqueous Solubility Prediction Method
logp	3.469		Crippen Method
mcvol	137.670	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
pc	2330.00	kPa	KDB
rinpol	785.50		NIST Webbook
rinpol	778.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	785.00		NIST Webbook

rinpol	776.00	NIST Webbook
rinpol	777.10	NIST Webbook
rinpol	782.00	NIST Webbook
rinpol	783.00	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	785.00	NIST Webbook
rinpol	785.10	NIST Webbook
rinpol	785.00	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	786.00	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	784.80	NIST Webbook
rinpol	785.30	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	786.10	NIST Webbook
rinpol	786.70	NIST Webbook
rinpol	787.20	NIST Webbook
rinpol	784.70	NIST Webbook
rinpol	784.40	NIST Webbook
rinpol	784.30	NIST Webbook
rinpol	784.10	NIST Webbook
rinpol	783.90	NIST Webbook
rinpol	783.60	NIST Webbook
rinpol	777.40	NIST Webbook
rinpol	777.00	NIST Webbook
rinpol	777.30	NIST Webbook
rinpol	774.90	NIST Webbook
rinpol	792.50	NIST Webbook
rinpol	778.00	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	785.00	NIST Webbook
rinpol	776.70	NIST Webbook
rinpol	786.00	NIST Webbook
rinpol	779.00	NIST Webbook
rinpol	783.00	NIST Webbook
rinpol	778.00	NIST Webbook
rinpol	777.00	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	776.50	NIST Webbook
rinpol	775.00	NIST Webbook

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rinpol	779.00	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	777.00	NIST Webbook
rinpol	778.00	NIST Webbook
rinpol	781.00	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	782.90	NIST Webbook
rinpol	786.00	NIST Webbook
rinpol	777.00	NIST Webbook
rinpol	789.00	NIST Webbook
rinpol	787.10	NIST Webbook
rinpol	780.10	NIST Webbook
rinpol	785.50	NIST Webbook
rinpol	782.21	NIST Webbook
rinpol	783.56	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	783.00	NIST Webbook
rinpol	786.60	NIST Webbook
rinpol	783.30	NIST Webbook
rinpol	784.80	NIST Webbook
rinpol	782.00	NIST Webbook
rinpol	797.06	NIST Webbook
rinpol	786.00	NIST Webbook
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rinpol	777.00	NIST Webbook
rinpol	791.00	NIST Webbook
rinpol	786.00	NIST Webbook
rinpol	782.00	NIST Webbook
rinpol	791.00	NIST Webbook
rinpol	781.00	NIST Webbook
rinpol	786.00	NIST Webbook
rinpol	795.00	NIST Webbook
rinpol	785.00	NIST Webbook
rinpol	773.00	NIST Webbook

rinpol	783.00		NIST Webbook
rinpol	778.00		NIST Webbook
tb	397.21 ± 0.20	K	NIST Webbook
tb	397.24 ± 0.40	K	NIST Webbook
tb	396.15 ± 1.00	K	NIST Webbook
tb	396.15 ± 1.00	K	NIST Webbook
tb	395.15 ± 1.50	K	NIST Webbook
tb	397.24 ± 0.20	K	NIST Webbook
tb	397.15 ± 0.20	K	NIST Webbook
tb	397.24	K	KDB
tb	397.30	K	NIST Webbook
tb	397.21 ± 0.20	K	NIST Webbook
tb	394.65 ± 1.50	K	NIST Webbook
tb	397.25 ± 0.40	K	NIST Webbook
tb	396.15 ± 2.00	K	NIST Webbook
tb	395.65 ± 2.00	K	NIST Webbook
tb	395.65 ± 3.00	K	NIST Webbook
tb	397.23 ± 0.03	K	NIST Webbook
tb	396.40 ± 0.60	K	NIST Webbook
tb	397.25 ± 0.50	K	NIST Webbook
tb	397.24 ± 0.10	K	NIST Webbook
tb	397.20	K	NIST Webbook
tc	569.80	K	KDB
tc	569.80 ± 2.00	K	NIST Webbook
tc	569.90 ± 2.00	K	NIST Webbook
tf	167.39	K	KDB
tf	167.30	K	Aqueous Solubility Prediction Method
vc	0.519	m3/kmol	KDB
zc	0.2552490		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.18	J/mol×K	549.55	Joback Method
cpg	319.96	J/mol×K	490.39	Joback Method
cpg	305.33	J/mol×K	460.81	Joback Method
cpg	289.98	J/mol×K	431.23	Joback Method
cpg	273.89	J/mol×K	401.65	Joback Method
cpg	359.82	J/mol×K	579.13	Joback Method
cpg	333.90	J/mol×K	519.97	Joback Method

dvisc	0.0055664	Pa×s	215.78	Joback Method
dvisc	0.0020930	Pa×s	252.96	Joback Method
dvisc	0.0010112	Pa×s	290.13	Joback Method
dvisc	0.0005763	Pa×s	327.30	Joback Method
dvisc	0.0003684	Pa×s	364.48	Joback Method
dvisc	0.0222427	Pa×s	178.61	Joback Method
dvisc	0.0002558	Pa×s	401.65	Joback Method
hvapt	33.65	kJ/mol	397.20	NIST Webbook
hvapt	33.77	kJ/mol	397.20	KDB
hvapt	38.50	kJ/mol	358.50	NIST Webbook
hvapt	41.10	kJ/mol	270.50	NIST Webbook
hvapt	40.10	kJ/mol	343.50	NIST Webbook
rfi	1.39728		298.15	KDB
rhoI	717.00	kg/m3	289.00	KDB
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42444e+01
Coeff. B	-3.40325e+03
Coeff. C	-4.36950e+01
Temperature range (K), min.	287.54
Temperature range (K), max.	424.67

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	7.84648e+01
Coeff. B	-7.31890e+03
Coeff. C	-9.41504e+00
Coeff. D	5.73647e-06
Temperature range (K), min.	167.39
Temperature range (K), max.	568.05

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3522949&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
KDB Pure (Korean Thermophysical Properties Databank):	https://www.thermoflow.com/research/kdb/hcprop/showprop.php?cmpid=84
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB:	https://www.thermoflow.com/files/research/kdb/mol/mol84.mol
KDB Vapor Pressure Data:	https://www.thermoflow.com/research/kdb/hcprop/showprop.php?cmpid=84

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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rho:	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

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