Hexane, 3,4-dimethyl-

Other names:	3,4-Dimethylhexane
	C2H5CH(CH3)CH(CH3)C2H5
Inchi:	InChI=1S/C8H18/c1-5-7(3)8(4)6-2/h7-8H,5-6H2,1-4H3
InchiKey:	RNTWWGNZUXGTAX-UHFFFAOYSA-N
Formula:	C8H18
SMILES:	CCC(C)C(C)CC
Mol. weight [g/mol]:	114.23
CAS:	583-48-2

Physical Properties

Property code	Value	Unit	Source
af	0.3380		KDB
ap	341.150	K	KDB
chl	-5468.70 ± 1.50	kJ/mol	NIST Webbook
chl	-5437.90	kJ/mol	NIST Webbook
gf	17.33	kJ/mol	KDB
hcg	5468.66	kJ/mol	KDB
hcn	5072.514	kJ/mol	KDB
hf	-213.00 ± 1.50	kJ/mol	NIST Webbook
hf	-213.10	kJ/mol	KDB
hfl	-252.00 ± 1.50	kJ/mol	NIST Webbook
hfus	9.43	kJ/mol	Joback Method
hvap	39.00 ± 0.10	kJ/mol	NIST Webbook
hvap	33.00	kJ/mol	NIST Webbook
hvap	38.97	kJ/mol	NIST Webbook
hvap	39.03	kJ/mol	NIST Webbook
log10ws	-2.69		Crippen Method
logp	3.079		Crippen Method
mcvol	123.580	ml/mol	McGowan Method
pc	2690.00 ± 40.00	kPa	NIST Webbook
pc	2692.10 ± 40.53	kPa	NIST Webbook
pc	2690.00	kPa	KDB
rhoc	244.45 ± 4.57	kg/m3	NIST Webbook
rhoc	244.45 ± 4.57	kg/m3	NIST Webbook
rinpol	769.60		NIST Webbook
rinpol	767.00		NIST Webbook
rinpol	772.00		NIST Webbook

rinpol	774.00	NIST Webbook
rinpol	771.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	768.00	NIST Webbook
rinpol	765.00	NIST Webbook
rinpol	770.00	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	770.00	NIST Webbook
rinpol	770.00	NIST Webbook
rinpol	768.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	770.20	NIST Webbook
rinpol	765.00	NIST Webbook
rinpol	767.70	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	765.00	NIST Webbook
rinpol	780.30	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	765.00	NIST Webbook
rinpol	774.70	NIST Webbook
rinpol	768.00	NIST Webbook
rinpol	770.50	NIST Webbook
rinpol	770.50	NIST Webbook
rinpol	770.60	NIST Webbook
rinpol	770.50	NIST Webbook
rinpol	770.60	NIST Webbook
rinpol	780.10	NIST Webbook
rinpol	780.00	NIST Webbook
rinpol	771.00	NIST Webbook
rinpol	771.00	NIST Webbook
rinpol	769.00	NIST Webbook
rinpol	771.10	NIST Webbook
rinpol	770.60	NIST Webbook
rinpol	772.60	NIST Webbook
rinpol	767.00	NIST Webbook
rinpol	769.00	NIST Webbook
rinpol	771.00	NIST Webbook
rinpol	770.10	NIST Webbook
rinpol	772.90	NIST Webbook
rinpol	768.40	NIST Webbook
rinpol	769.30	NIST Webbook
rinpol	770.20	NIST Webbook
rinpol	771.20	NIST Webbook

rinpol	766.00	NIST Webbook
rinpol	767.00	NIST Webbook
rinpol	768.00	NIST Webbook
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rinpol	770.00	NIST Webbook
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rinpol	773.00	NIST Webbook
rinpol	770.00	NIST Webbook
rinpol	771.00	NIST Webbook
rinpol	773.00	NIST Webbook

rinpol	764.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	767.20		NIST Webbook
rinpol	770.20		NIST Webbook
rinpol	764.08		NIST Webbook
rinpol	767.60		NIST Webbook
rinpol	765.50		NIST Webbook
rinpol	768.08		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	766.04		NIST Webbook
rinpol	767.33		NIST Webbook
rinpol	768.12		NIST Webbook
rinpol	766.33		NIST Webbook
rinpol	767.70		NIST Webbook
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rinpol	771.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	772.00		NIST Webbook
tb	391.15 ± 1.00	K	NIST Webbook
tb	390.88	K	KDB
tb	390.90	K	NIST Webbook
tb	390.90	K	NIST Webbook
tb	389.65 ± 0.50	K	NIST Webbook
tb	389.65 ± 0.60	K	NIST Webbook
tb	391.05 ± 0.20	K	NIST Webbook
tb	391.00 ± 0.30	K	NIST Webbook
tb	391.15 ± 0.30	K	NIST Webbook
tb	390.87 ± 0.10	K	NIST Webbook
tb	390.55 ± 0.30	K	NIST Webbook
tb	390.55 ± 0.30	K	NIST Webbook
tb	390.89 ± 0.30	K	NIST Webbook
tb	390.78 ± 0.40	K	NIST Webbook
tb	390.87 ± 0.01	K	NIST Webbook
tb	391.15 ± 0.50	K	NIST Webbook
tb	390.60 ± 0.15	K	NIST Webbook
tb	391.15 ± 1.00	K	NIST Webbook
tb	390.20 ± 0.30	K	NIST Webbook
tb	390.88 ± 0.20	K	NIST Webbook

tb	390.91 ± 0.10	K	NIST Webbook
tb	391.90 ± 0.50	K	NIST Webbook
tc	568.80	K	NIST Webbook
tc	568.78 ± 0.40	K	NIST Webbook
tc	568.80	K	KDB
tc	568.80 ± 0.50	K	NIST Webbook
tf	149.92	K	Joback Method
vc	0.466	m3/kmol	KDB
vc	0.466	m3/kmol	NIST Webbook
zc	0.2650590		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.18	J/mol×K	406.70	NIST Webbook
cpg	272.38	J/mol×K	462.30	NIST Webbook
cpg	300.41	J/mol×K	522.60	NIST Webbook
dvisc	0.0008449	Pa×s	265.74	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	0.0048914	Pa×s	188.53	Joback Method
dvisc	0.0017511	Pa×s	227.13	Joback Method
dvisc	0.0231912	Pa×s	149.92	Joback Method
hvapt	41.30	kJ/mol	320.50	NIST Webbook
hvapt	37.70	kJ/mol	352.50	NIST Webbook
hvapt	33.27	kJ/mol	391.90	KDB
hvapt	33.24	kJ/mol	390.90	NIST Webbook
rfi	1.40180		298.15	KDB
rhol	719.00	kg/m3	293.00	KDB
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41933e+01

Coeff. B	-3.27107e+03
Coeff. C	-4.92520e+01
Temperature range (K), min.	284.48
Temperature range (K), max.	417.54

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.76065e+01
Coeff. B	-7.55662e+03
Coeff. C	-1.08609e+01
Coeff. D	7.63359e-06
Temperature range (K), min.	250.00
Temperature range (K), max.	568.80

Sources

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=56
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Infinite dilution activity coefficients, specific retention volumes and solvation thermodynamics of hydrocarbons in C78H158 branched alkane solvent:	https://www.doi.org/10.1016/j.fluid.2006.07.015
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=56
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C583482&Units=SI
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
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility