Hexane, 2,2-dimethyl-

Other names:	(CH3)3C(CH2)3CH3
	2,2-Dimethylhexane
Inchi:	InChI=1S/C8H18/c1-5-6-7-8(2,3)4/h5-7H2,1-4H3
InchiKey:	FLTJDUOFAQWHDF-UHFFFAOYSA-N
Formula:	C8H18
SMILES:	CCCCC(C)(C)C
Mol. weight [g/mol]:	114.23
CAS:	590-73-8

Physical Properties

Property code	Value	Unit	Source
af	0.3380		KDB
ap	351.150	K	KDB
chl	-5458.61 ± 0.88	kJ/mol	NIST Webbook
gf	10.72	kJ/mol	KDB
hcg	5458.61	kJ/mol	KDB
hcn	5062.473	kJ/mol	KDB
hf	-224.90	kJ/mol	KDB
hf	-224.70 ± 1.00	kJ/mol	NIST Webbook
hfl	-262.00 ± 1.00	kJ/mol	NIST Webbook
hfus	9.06	kJ/mol	Joback Method
hvap	37.30	kJ/mol	NIST Webbook
hvap	37.36	kJ/mol	NIST Webbook
hvap	37.29	kJ/mol	NIST Webbook
hvap	37.30 ± 0.10	kJ/mol	NIST Webbook
log10ws	-2.93		Crippen Method
logp	3.223		Crippen Method
mcvol	123.580	ml/mol	McGowan Method
pc	2530.00	kPa	KDB
pc	2529.20 ± 40.53	kPa	NIST Webbook
pc	2530.00 ± 40.00	kPa	NIST Webbook
rhoc	238.74 ± 4.57	kg/m3	NIST Webbook
rhoc	238.74 ± 4.57	kg/m3	NIST Webbook
rinpol	722.90		NIST Webbook
rinpol	718.00		NIST Webbook
rinpol	720.10		NIST Webbook
rinpol	720.90		NIST Webbook

rinpol	723.90	NIST Webbook
rinpol	719.00	NIST Webbook
rinpol	719.27	NIST Webbook
rinpol	718.82	NIST Webbook
rinpol	722.00	NIST Webbook
rinpol	719.00	NIST Webbook
rinpol	723.00	NIST Webbook
rinpol	724.00	NIST Webbook
rinpol	722.00	NIST Webbook
rinpol	720.00	NIST Webbook
rinpol	715.00	NIST Webbook
rinpol	720.00	NIST Webbook
rinpol	723.00	NIST Webbook
rinpol	720.00	NIST Webbook
rinpol	721.00	NIST Webbook
rinpol	719.00	NIST Webbook
rinpol	717.90	NIST Webbook
rinpol	720.00	NIST Webbook
rinpol	720.00	NIST Webbook
rinpol	722.00	NIST Webbook
rinpol	717.00	NIST Webbook
rinpol	721.60	NIST Webbook
rinpol	722.50	NIST Webbook
rinpol	720.40	NIST Webbook
rinpol	713.00	NIST Webbook
rinpol	718.00	NIST Webbook
rinpol	721.00	NIST Webbook
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rinpol	716.00	NIST Webbook
rinpol	719.40	NIST Webbook
rinpol	720.00	NIST Webbook
rinpol	718.00	NIST Webbook
rinpol	721.30	NIST Webbook
rinpol	718.00	NIST Webbook
rinpol	722.90	NIST Webbook
rinpol	722.80	NIST Webbook

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rinpol	722.80	NIST Webbook
rinpol	723.20	NIST Webbook
rinpol	719.00	NIST Webbook
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rinpol	722.10	NIST Webbook
rinpol	723.80	NIST Webbook
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rinpol	723.00	NIST Webbook
rinpol	726.00	NIST Webbook
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rinpol	720.00	NIST Webbook
rinpol	725.75	NIST Webbook
rinpol	726.42	NIST Webbook
rinpol	727.80	NIST Webbook
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rinpol	717.00		NIST Webbook
rinpol	719.70		NIST Webbook
rinpol	720.00		NIST Webbook
rinpol	720.00		NIST Webbook
rinpol	720.00		NIST Webbook
rinpol	721.00		NIST Webbook
rinpol	718.00		NIST Webbook
rinpol	722.00		NIST Webbook
rinpol	719.00		NIST Webbook
rinpol	718.00		NIST Webbook
rinpol	720.00		NIST Webbook
rinpol	720.00		NIST Webbook
rinpol	721.00		NIST Webbook
rinpol	718.50		NIST Webbook
rinpol	718.00		NIST Webbook
tb	380.05 ± 0.30	K	NIST Webbook
tb	380.01	K	KDB
tb	380.00	K	NIST Webbook
tb	382.00	K	NIST Webbook
tb	379.95 ± 0.30	K	NIST Webbook
tb	379.00 ± 2.00	K	NIST Webbook
tb	379.99 ± 0.20	K	NIST Webbook
tb	380.20 ± 0.50	K	NIST Webbook
tb	380.01 ± 0.20	K	NIST Webbook
tb	380.00 ± 0.30	K	NIST Webbook
tb	380.15 ± 0.50	K	NIST Webbook
tb	379.65 ± 0.40	K	NIST Webbook
tb	380.00 ± 0.50	K	NIST Webbook
tb	379.99 ± 0.01	K	NIST Webbook
tb	379.65 ± 1.50	K	NIST Webbook
tb	380.10 ± 0.60	K	NIST Webbook
tb	379.35 ± 0.50	K	NIST Webbook
tb	379.95 ± 0.40	K	NIST Webbook
tb	379.99 ± 0.10	K	NIST Webbook
tb	380.15 ± 1.00	K	NIST Webbook
tb	380.25 ± 0.50	K	NIST Webbook
tb	380.01 ± 0.30	K	NIST Webbook
tb	380.01 ± 0.30	K	NIST Webbook
tb	380.03 ± 0.20	K	NIST Webbook
tc	549.80 ± 0.50	K	NIST Webbook

tc	549.80 ± 0.40	K	NIST Webbook
tc	549.80	K	KDB
tf	151.97	K	KDB
tf	151.97 ± 0.10	K	NIST Webbook
tf	152.00 ± 0.08	K	NIST Webbook
tf	151.97 ± 0.03	K	NIST Webbook
tf	151.59 ± 0.20	K	NIST Webbook
tf	151.91 ± 0.01	K	NIST Webbook
tf	151.90 ± 0.06	K	NIST Webbook
tf	151.97 ± 0.04	K	NIST Webbook
tf	151.88 ± 0.08	K	NIST Webbook
tf	151.93 ± 0.06	K	NIST Webbook
tf	151.94 ± 0.05	K	NIST Webbook
vc	0.478	m3/kmol	NIST Webbook
vc	0.478	m3/kmol	KDB
zc	0.2645500		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.30	J/mol×K	553.39	Joback Method
cpg	287.68	J/mol×K	495.33	Joback Method
cpg	275.00	J/mol×K	466.30	Joback Method
cpg	261.70	J/mol×K	437.27	Joback Method
cpg	247.76	J/mol×K	408.24	Joback Method
cpg	233.16	J/mol×K	379.21	Joback Method
cpg	299.78	J/mol×K	524.36	Joback Method
dvisc	0.0038192	Pa×s	215.15	Joback Method
dvisc	0.0017124	Pa×s	247.96	Joback Method
dvisc	0.0009261	Pa×s	280.77	Joback Method
dvisc	0.0005696	Pa×s	313.59	Joback Method
dvisc	0.0003841	Pa×s	346.40	Joback Method
dvisc	0.0113690	Pa×s	182.34	Joback Method
dvisc	0.0002773	Pa×s	379.21	Joback Method
hvapt	32.26	kJ/mol	380.00	KDB
hvapt	39.70	kJ/mol	311.50	NIST Webbook
hvapt	36.60	kJ/mol	341.50	NIST Webbook
hvapt	32.07	kJ/mol	382.00	NIST Webbook
rfi	1.39104		298.15	KDB
rhol	695.00	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	1.42379e+01
Coeff. B	-3.25003e+03
Coeff. C	-4.21330e+01
Temperature range (K), min.	275.11
Temperature range (K), max.	406.23

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.72842e+01
Coeff. B	-7.33307e+03
Coeff. C	-1.08622e+01
Coeff. D	8.00732e-06
Temperature range (K), min.	151.97
Temperature range (K), max.	549.80

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=51
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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol51.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C590738&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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