

Hexane, 2,4-dimethyl-

Other names:	2,4-Dimethylhexane
Inchi:	InChI=1S/C8H18/c1-5-8(4)6-7(2)3/h7-8H,5-6H2,1-4H3
InchiKey:	HDGQICNBXPAKLR-UHFFFAOYSA-N
Formula:	C8H18
SMILES:	CCC(C)CC(C)C
Mol. weight [g/mol]:	114.23
CAS:	589-43-5

Physical Properties

Property code	Value	Unit	Source
af	0.3430		KDB
ap	346.550	K	KDB
chl	-5266.20	kJ/mol	NIST Webbook
chl	-5463.50 ± 1.00	kJ/mol	NIST Webbook
gf	11.72	kJ/mol	KDB
hcg	5463.47	kJ/mol	KDB
hcn	5067.326	kJ/mol	KDB
hf	-219.40 ± 1.10	kJ/mol	NIST Webbook
hf	-219.60	kJ/mol	KDB
hfl	-257.20 ± 1.10	kJ/mol	NIST Webbook
hfus	9.43	kJ/mol	Joback Method
hvap	37.76	kJ/mol	NIST Webbook
hvap	37.80 ± 0.10	kJ/mol	NIST Webbook
hvap	37.83	kJ/mol	NIST Webbook
hvap	37.80	kJ/mol	NIST Webbook
log10ws	-2.69		Crippen Method
logp	3.079		Crippen Method
mcvol	123.580	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
pc	2560.00 ± 40.00	kPa	NIST Webbook
pc	2560.00	kPa	KDB
pc	2487.80 ± 7.50	kPa	NIST Webbook
pc	2556.30 ± 40.53	kPa	NIST Webbook
rhoc	242.16 ± 4.57	kg/m3	NIST Webbook
rhoc	242.16 ± 4.57	kg/m3	NIST Webbook
rinpol	736.00		NIST Webbook
rinpol	733.00		NIST Webbook

rinpol	731.00	NIST Webbook
rinpol	732.00	NIST Webbook
rinpol	733.00	NIST Webbook
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rinpol	724.00	NIST Webbook
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rinpol	735.00	NIST Webbook
rinpol	728.00	NIST Webbook
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rinpol	735.00		NIST Webbook
rinpol	734.00		NIST Webbook
rinpol	733.00		NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	736.00		NIST Webbook
rinpol	735.00		NIST Webbook
tb	382.58 ± 0.20	K	NIST Webbook
tb	382.60	K	KDB

tb	382.60	K	NIST Webbook
tb	380.00 ± 3.00	K	NIST Webbook
tb	380.00 ± 3.00	K	NIST Webbook
tb	382.64 ± 0.10	K	NIST Webbook
tb	382.59 ± 0.20	K	NIST Webbook
tb	381.40 ± 1.50	K	NIST Webbook
tb	383.05 ± 1.00	K	NIST Webbook
tb	383.05 ± 0.60	K	NIST Webbook
tb	382.35 ± 0.50	K	NIST Webbook
tb	382.65 ± 0.50	K	NIST Webbook
tb	382.95 ± 0.20	K	NIST Webbook
tb	383.15 ± 2.00	K	NIST Webbook
tb	382.65 ± 0.20	K	NIST Webbook
tb	382.65 ± 0.20	K	NIST Webbook
tb	382.57 ± 0.01	K	NIST Webbook
tb	382.95 ± 0.50	K	NIST Webbook
tb	382.50 ± 0.15	K	NIST Webbook
tb	382.95 ± 0.30	K	NIST Webbook
tb	382.15 ± 2.00	K	NIST Webbook
tb	382.25 ± 0.50	K	NIST Webbook
tb	382.58 ± 0.10	K	NIST Webbook
tc	553.50	K	KDB
tc	553.50 ± 0.50	K	NIST Webbook
tc	553.45 ± 0.40	K	NIST Webbook
tc	550.00 ± 1.00	K	NIST Webbook
tf	149.92	K	Joback Method
vc	0.472	m3/kmol	KDB
vc	0.472	m3/kmol	NIST Webbook
zc	0.2625590		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.00	J/mol×K	381.56	Joback Method
cpg	259.09	J/mol×K	438.59	Joback Method
cpg	307.33	J/mol×K	552.64	Joback Method
cpg	271.88	J/mol×K	467.10	Joback Method
cpg	284.17	J/mol×K	495.62	Joback Method
cpg	295.99	J/mol×K	524.13	Joback Method
cpg	245.80	J/mol×K	410.07	Joback Method
dvisc	0.0003218	Pa×s	342.95	Joback Method

dvisc	0.0004905	Pa×s	304.35	Joback Method
dvisc	0.0008449	Pa×s	265.74	Joback Method
dvisc	0.0017511	Pa×s	227.13	Joback Method
dvisc	0.0048914	Pa×s	188.53	Joback Method
dvisc	0.0002299	Pa×s	381.56	Joback Method
dvisc	0.0231912	Pa×s	149.92	Joback Method
hvapt	41.00	kJ/mol	314.00	NIST Webbook
hvapt	36.90	kJ/mol	345.00	NIST Webbook
hvapt	32.51	kJ/mol	382.60	NIST Webbook
hvapt	32.59	kJ/mol	382.80	KDB
rfi	1.39291		298.15	KDB
rhoI	700.00	kg/m3	293.00	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	1.41448e+01
Coeff. B	-3.17490e+03
Coeff. C	-4.93070e+01
Temperature range (K), min.	278.42
Temperature range (K), max.	408.73

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	8.77418e+01
Coeff. B	-7.41293e+03
Coeff. C	-1.09146e+01
Coeff. D	7.94824e-06
Temperature range (K), min.	245.00
Temperature range (K), max.	553.50

Sources

KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=53
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Infinite dilution activity coefficients, specific retention volumes and solvent thermodynamics of hydrocarbons in C7H158 branched alkane solvent:	https://www.doi.org/10.1016/j.fluid.2006.07.015
Joback Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The Yaws Handbook of Vapor Pressure:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://link.springer.com/article/10.1007/BF02311772
KDB:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C589435&Units=SI
	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=53

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
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhoc:	Critical density
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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