Hexane, 2,5-dimethyl-

Other names:	2,5-Dimethylhexane
	BIISOBUTYL
Inchi:	InChI=1S/C8H18/c1-7(2)5-6-8(3)4/h7-8H,5-6H2,1-4H3
InchiKey:	UWNADWZGEHDQAB-UHFFFAOYSA-N
Formula:	C8H18
SMILES:	CC(C)CCC(C)C
Mol. weight [g/mol]:	114.23
CAS:	592-13-2

Physical Properties

Property code	Value	Unit	Source
af	0.3560		KDB
ap	351.150	K	KDB
chl	-5460.10 ± 1.40	kJ/mol	NIST Webbook
chl	-5266.20	kJ/mol	NIST Webbook
chl	-5435.90	kJ/mol	NIST Webbook
gf	10.47	kJ/mol	KDB
hcg	5460.12	kJ/mol	KDB
hcn	5063.979	kJ/mol	KDB
hf	-222.60 ± 1.50	kJ/mol	NIST Webbook
hf	-222.80	kJ/mol	KDB
hfl	-260.50 ± 1.50	kJ/mol	NIST Webbook
hfus	9.43	kJ/mol	Joback Method
hvap	37.92	kJ/mol	NIST Webbook
hvap	37.90 ± 0.10	kJ/mol	NIST Webbook
hvap	37.85	kJ/mol	NIST Webbook
hvap	37.90	kJ/mol	NIST Webbook
hvap	32.00	kJ/mol	NIST Webbook
ie	9.76	eV	NIST Webbook
log10ws	-2.69		Crippen Method
logp	3.079		Crippen Method
mcvol	123.580	ml/mol	McGowan Method
pc	2490.00	kPa	KDB
pc	2486.70 ± 40.53	kPa	NIST Webbook
pc	2490.00 ± 20.00	kPa	NIST Webbook
pc	2487.80 ± 20.00	kPa	NIST Webbook
rhoc	236.45 ± 4.57	kg/m3	NIST Webbook

rhoc	236.57 ± 2.28	kg/m3	NIST Webbook
rhoc	236.45 ± 2.28	kg/m3	NIST Webbook
rinpol	728.00		NIST Webbook
rinpol	730.40		NIST Webbook
rinpol	729.00		NIST Webbook
rinpol	733.00		NIST Webbook
rinpol	728.00		NIST Webbook
rinpol	732.30		NIST Webbook
rinpol	732.00		NIST Webbook
rinpol	731.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	729.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	729.00		NIST Webbook
rinpol	728.00		NIST Webbook
rinpol	733.00		NIST Webbook
rinpol	732.00		NIST Webbook
rinpol	732.00		NIST Webbook
rinpol	732.00		NIST Webbook
rinpol	733.00		NIST Webbook
rinpol	729.00		NIST Webbook
rinpol	722.00		NIST Webbook
rinpol	729.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	732.00		NIST Webbook
rinpol	732.00		NIST Webbook
rinpol	728.00		NIST Webbook
rinpol	733.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	736.30		NIST Webbook
rinpol	732.50		NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	728.00		NIST Webbook
rinpol	729.00		NIST Webbook
rinpol	728.09		NIST Webbook
rinpol	728.00		NIST Webbook
rinpol	726.90		NIST Webbook
rinpol	726.90		NIST Webbook
rinpol	729.70		NIST Webbook
rinpol	727.54		NIST Webbook
rinpol	727.10		NIST Webbook
rinpol	732.00		NIST Webbook
rinpol	735.00		NIST Webbook

rinpol	730.00	NIST Webbook
rinpol	721.00	NIST Webbook
rinpol	727.00	NIST Webbook
rinpol	727.00	NIST Webbook
rinpol	729.00	NIST Webbook
rinpol	730.00	NIST Webbook
rinpol	729.00	NIST Webbook
rinpol	729.00	NIST Webbook
rinpol	731.00	NIST Webbook
rinpol	728.00	NIST Webbook
rinpol	733.20	NIST Webbook
rinpol	732.00	NIST Webbook
rinpol	730.00	NIST Webbook
rinpol	726.00	NIST Webbook
rinpol	730.40	NIST Webbook
rinpol	731.00	NIST Webbook
rinpol	731.00	NIST Webbook
rinpol	732.00	NIST Webbook
rinpol	730.70	NIST Webbook
rinpol	732.30	NIST Webbook
rinpol	734.50	NIST Webbook
rinpol	727.00	NIST Webbook
rinpol	732.50	NIST Webbook
rinpol	732.40	NIST Webbook
rinpol	732.50	NIST Webbook
rinpol	732.40	NIST Webbook
rinpol	732.80	NIST Webbook
rinpol	731.00	NIST Webbook
rinpol	732.00	NIST Webbook
rinpol	733.00	NIST Webbook
rinpol	733.00	NIST Webbook
rinpol	728.40	NIST Webbook
rinpol	729.00	NIST Webbook
rinpol	731.00	NIST Webbook
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rinpol	732.00	NIST Webbook
rinpol	728.00	NIST Webbook
rinpol	729.30	NIST Webbook
rinpol	728.00	NIST Webbook
rinpol	728.00	NIST Webbook
rinpol	729.00	NIST Webbook
rinpol	732.60	NIST Webbook
rinpol	732.80	NIST Webbook
rinpol	733.00	NIST Webbook

rinpol	733.20		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	731.00		NIST Webbook
rinpol	731.00		NIST Webbook
rinpol	731.00		NIST Webbook
rinpol	732.00		NIST Webbook
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rinpol	723.00		NIST Webbook
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rinpol	728.00		NIST Webbook
rinpol	729.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	728.00		NIST Webbook
ripol	742.00		NIST Webbook
tb	382.15 ± 1.00	K	NIST Webbook

tb	382.27	K	KDB
tb	381.20	K	NIST Webbook
tb	382.20 ± 0.30	K	NIST Webbook
tb	382.30	K	NIST Webbook
tb	381.50 ± 0.50	K	NIST Webbook
tb	382.30	K	NIST Webbook
tb	382.25 ± 0.20	K	NIST Webbook
tb	382.25 ± 1.00	K	NIST Webbook
tb	382.55 ± 0.40	K	NIST Webbook
tb	382.30 ± 0.20	K	NIST Webbook
tb	382.35 ± 0.30	K	NIST Webbook
tb	382.45 ± 0.30	K	NIST Webbook
tb	382.15 ± 0.30	K	NIST Webbook
tb	382.30 ± 0.30	K	NIST Webbook
tb	382.35 ± 0.30	K	NIST Webbook
tb	382.60 ± 0.50	K	NIST Webbook
tb	382.45 ± 0.50	K	NIST Webbook
tb	382.25 ± 0.01	K	NIST Webbook
tb	381.30 ± 0.60	K	NIST Webbook
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tb	382.35 ± 0.50	K	NIST Webbook
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tb	381.65 ± 1.00	K	NIST Webbook
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tb	382.55 ± 0.30	K	NIST Webbook
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tb	382.65 ± 0.50	K	NIST Webbook
tb	382.45 ± 0.20	K	NIST Webbook
tb	382.40 ± 0.30	K	NIST Webbook
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tb	382.45 ± 0.20	K	NIST Webbook
tb	382.45 ± 0.50	K	NIST Webbook
tb	382.45 ± 0.50	K	NIST Webbook
tb	382.25 ± 0.10	K	NIST Webbook
tb	382.35 ± 0.20	K	NIST Webbook
tb	382.35 ± 0.20	K	NIST Webbook
tb	382.27 ± 0.10	K	NIST Webbook
tc	550.00 ± 0.50	K	NIST Webbook
tc	544.00 ± 8.00	K	NIST Webbook
tc	550.50	K	KDB
tc	550.00 ± 0.50	K	NIST Webbook
tc	549.99 ± 0.40	K	NIST Webbook

tf	181.94 ± 0.20	K	NIST Webbook
tf	181.66 ± 0.30	K	NIST Webbook
tf	181.66 ± 0.20	K	NIST Webbook
tf	181.74 ± 0.01	K	NIST Webbook
tf	181.88 ± 0.07	K	NIST Webbook
tf	181.89 ± 0.05	K	NIST Webbook
tf	181.66 ± 0.30	K	NIST Webbook
tf	181.96 ± 0.20	K	NIST Webbook
tf	181.66 ± 0.50	K	NIST Webbook
tf	182.95 ± 0.50	K	NIST Webbook
tf	183.05 ± 0.30	K	NIST Webbook
tf	180.45 ± 0.30	K	NIST Webbook
tf	179.15 ± 2.00	K	NIST Webbook
tf	181.94 ± 0.30	K	NIST Webbook
tf	179.15 ± 0.20	K	NIST Webbook
tf	182.08 ± 0.40	K	NIST Webbook
tf	182.45 ± 0.30	K	NIST Webbook
tf	181.95 ± 0.03	K	NIST Webbook
tf	182.00	K	KDB
tf	181.85 ± 0.40	K	NIST Webbook
tt	181.96 ± 0.04	K	NIST Webbook
tt	181.97 ± 0.02	K	NIST Webbook
tt	181.96 ± 0.04	K	NIST Webbook
vc	0.482	m3/kmol	KDB
vc	0.482	m3/kmol	NIST Webbook
zc	0.2622120		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.99	J/mol×K	524.13	Joback Method
cpg	284.17	J/mol×K	495.62	Joback Method
cpg	307.33	J/mol×K	552.64	Joback Method
cpg	232.00	J/mol×K	381.56	Joback Method
cpg	245.80	J/mol×K	410.07	Joback Method
cpg	259.09	J/mol×K	438.59	Joback Method
cpg	271.88	J/mol×K	467.10	Joback Method
cpl	249.20	J/mol×K	298.15	NIST Webbook
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	0.0231912	Pa×s	149.92	Joback Method
dvisc	0.0048914	Pa×s	188.53	Joback Method
dvisc	0.0017511	Pa×s	227.13	Joback Method
dvisc	0.0008449	Pa×s	265.74	Joback Method
hvapt	41.10	kJ/mol	314.00	NIST Webbook
hvapt	32.54	kJ/mol	382.30	NIST Webbook
hvapt	36.90	kJ/mol	345.00	NIST Webbook
hvapt	32.63	kJ/mol	381.80	KDB
rfi	1.39004		298.15	KDB
rhol	693.00	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	1.42275e+01
Coeff. B	-3.22571e+03
Coeff. C	-4.65690e+01
Temperature range (K), min.	277.97
Temperature range (K), max.	408.36

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.97264e+01
Coeff. B	-7.50283e+03
Coeff. C	-1.12156e+01
Coeff. D	8.24692e-06
Temperature range (K), min.	182.00
Temperature range (K), max.	550.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Solubility of CO2 in branched alkanes in order to extend the PPR78 model (predictive 1978, Peng Robinson EOS with temperature-dependent kij calculated through a group contribution method) to such systems:	https://www.doi.org/10.1016/j.fluid.2005.10.001

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=54
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol54.mol
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C592132&Units=SI

Legend

af:	Acentric Factor
ap:	Aniline Point
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
ie:	Ionization energy
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
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

zc: Critical Compressibility