

Hexane, 2,3-dimethyl-

Other names:	2,3-Dimethylhexane 2,3-Dimethylhexane
Inchi:	InChI=1S/C8H18/c1-5-6-8(4)7(2)3/h7-8H,5-6H2,1-4H3
InchiKey:	JXPOLSKBTUYKJB-UHFFFAOYSA-N
Formula:	C8H18
SMILES:	CCCC(C)C(C)C
Mol. weight [g/mol]:	114.23
CAS:	584-94-1

Physical Properties

Property code	Value	Unit	Source
af	0.3460		KDB
ap	343.750	K	KDB
chl	-5467.90 ± 1.40	kJ/mol	NIST Webbook
gf	17.71	kJ/mol	KDB
hcg	5467.90	kJ/mol	KDB
hcn	5071.762	kJ/mol	KDB
hf	-214.10	kJ/mol	KDB
hf	-213.90 ± 1.50	kJ/mol	NIST Webbook
hfl	-252.80 ± 1.50	kJ/mol	NIST Webbook
hfus	9.43	kJ/mol	Joback Method
hvap	38.83	kJ/mol	NIST Webbook
hvap	38.80	kJ/mol	NIST Webbook
hvap	38.80 ± 0.10	kJ/mol	NIST Webbook
hvap	38.79	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	2630.00 ± 40.00	kPa	NIST Webbook
pc	2628.20 ± 40.53	kPa	NIST Webbook
pc	2630.00	kPa	KDB
rhoc	244.45 ± 4.57	kg/m3	NIST Webbook
rhoc	244.45 ± 4.57	kg/m3	NIST Webbook
rinpol	762.00		NIST Webbook
rinpol	758.60		NIST Webbook
rinpol	761.40		NIST Webbook

rinpol	769.99	NIST Webbook
rinpol	761.00	NIST Webbook
rinpol	756.00	NIST Webbook
rinpol	760.00	NIST Webbook
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rinpol	759.00	NIST Webbook
rinpol	760.30	NIST Webbook
rinpol	761.00	NIST Webbook
rinpol	758.00	NIST Webbook
rinpol	761.00	NIST Webbook
rinpol	761.00	NIST Webbook
rinpol	763.00	NIST Webbook
rinpol	763.00	NIST Webbook
rinpol	762.00	NIST Webbook
rinpol	761.00	NIST Webbook
rinpol	761.00	NIST Webbook
rinpol	761.10	NIST Webbook
rinpol	758.00	NIST Webbook
rinpol	762.00	NIST Webbook
rinpol	760.00	NIST Webbook
rinpol	761.20	NIST Webbook
rinpol	763.66	NIST Webbook
rinpol	759.00	NIST Webbook
rinpol	755.00	NIST Webbook
rinpol	759.00	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	757.90	NIST Webbook
rinpol	760.50	NIST Webbook
rinpol	757.00	NIST Webbook
rinpol	761.00	NIST Webbook
rinpol	761.00	NIST Webbook
rinpol	752.00	NIST Webbook
rinpol	758.60	NIST Webbook
rinpol	760.20	NIST Webbook
rinpol	765.60	NIST Webbook
rinpol	761.00	NIST Webbook
rinpol	757.00	NIST Webbook
rinpol	761.40	NIST Webbook
rinpol	759.60	NIST Webbook
rinpol	758.00	NIST Webbook
rinpol	765.60	NIST Webbook
rinpol	761.00	NIST Webbook
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rinpol	762.20	NIST Webbook

rinpol	760.10	NIST Webbook
rinpol	761.50	NIST Webbook
rinpol	761.00	NIST Webbook
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rinpol	758.00	NIST Webbook
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rinpol	759.70	NIST Webbook
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rinpol	762.00		NIST Webbook
rinpol	762.00		NIST Webbook
rinpol	762.00		NIST Webbook
rinpol	757.00		NIST Webbook
tb	388.77	K	KDB
tb	388.80	K	NIST Webbook
tb	388.79 ± 0.10	K	NIST Webbook
tb	388.75 ± 0.20	K	NIST Webbook
tb	389.65 ± 2.00	K	NIST Webbook
tb	389.65 ± 2.00	K	NIST Webbook
tb	387.05 ± 0.50	K	NIST Webbook
tb	388.45 ± 0.80	K	NIST Webbook
tb	388.45 ± 0.50	K	NIST Webbook
tb	388.85 ± 0.50	K	NIST Webbook
tb	388.95 ± 0.20	K	NIST Webbook
tb	388.95 ± 0.50	K	NIST Webbook
tb	388.95 ± 0.30	K	NIST Webbook
tb	387.35 ± 1.00	K	NIST Webbook
tb	388.65 ± 0.60	K	NIST Webbook
tb	388.65 ± 0.20	K	NIST Webbook
tb	388.75 ± 0.10	K	NIST Webbook
tb	387.25 ± 1.00	K	NIST Webbook
tb	388.40 ± 0.60	K	NIST Webbook
tb	388.84 ± 0.30	K	NIST Webbook
tb	388.75 ± 0.01	K	NIST Webbook
tb	388.65 ± 0.40	K	NIST Webbook
tb	389.15 ± 1.00	K	NIST Webbook
tb	388.75 ± 0.30	K	NIST Webbook
tb	389.00 ± 0.30	K	NIST Webbook
tb	388.65 ± 0.30	K	NIST Webbook
tb	388.95 ± 0.20	K	NIST Webbook
tb	388.75 ± 0.30	K	NIST Webbook
tb	388.76 ± 0.20	K	NIST Webbook
tb	388.80	K	NIST Webbook
tc	563.50	K	KDB
tc	563.50 ± 0.50	K	NIST Webbook
tc	563.40	K	NIST Webbook
tc	563.42 ± 0.40	K	NIST Webbook
tf	149.92	K	Joback Method
vc	0.468	m3/kmol	KDB

vc	0.468	m3/kmol	NIST Webbook
zc	0.2627070		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.58	J/mol×K	397.40	NIST Webbook
cpg	273.22	J/mol×K	463.70	NIST Webbook
cpg	299.99	J/mol×K	522.20	NIST Webbook
dvisc	0.0004905	Pa×s	304.35	Joback Method
dvisc	0.0002299	Pa×s	381.56	Joback Method
dvisc	0.0003218	Pa×s	342.95	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	41.40	kJ/mol	319.00	NIST Webbook
hvapt	33.17	kJ/mol	388.80	NIST Webbook
hvapt	37.60	kJ/mol	350.00	NIST Webbook
hvapt	33.20	kJ/mol	388.80	KDB
rfi	1.39880		298.15	KDB
rhoI	712.00	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	1.41996e+01
Coeff. B	-3.24994e+03
Coeff. C	-4.95620e+01
Temperature range (K), min.	283.17
Temperature range (K), max.	415.21

Information	Value
Property code	pvap

Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	8.80002e+01
Coeff. B	-7.54302e+03
Coeff. C	-1.09261e+01
Coeff. D	7.76601e-06
Temperature range (K), min.	250.00
Temperature range (K), max.	563.40

Sources

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.thermo.com/research/kdb/hcprop/showprop.php?cmpid=52
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C584941&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=52

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
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

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