

1-Hexene, 4-methyl-

Other names:	4-Methyl-1-hexene 4-methylhex-1-ene C ₂ H ₅ CH(CH ₃)CH ₂ CH=CH ₂
Inchi:	InChI=1S/C ₇ H ₁₄ /c1-4-6-7(3)5-2/h4,7H,1,5-6H2,2-3H3
InchiKey:	SUWJESCICIOQHO-UHFFFAOYSA-N
Formula:	C ₇ H ₁₄
SMILES:	C=CCC(C)CC
Mol. weight [g/mol]:	98.19
CAS:	3769-23-1

Physical Properties

Property code	Value	Unit	Source
gf	93.46	kJ/mol	Joback Method
hf	-67.66	kJ/mol	Joback Method
hfus	9.08	kJ/mol	Joback Method
hvap	34.70	kJ/mol	NIST Webbook
log10ws	-2.36		Crippen Method
logp	2.609		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	657.00		NIST Webbook
rinpol	663.00		NIST Webbook
rinpol	664.00		NIST Webbook
rinpol	664.00		NIST Webbook
rinpol	660.00		NIST Webbook
rinpol	658.00		NIST Webbook
rinpol	659.30		NIST Webbook
rinpol	656.40		NIST Webbook
rinpol	658.00		NIST Webbook
rinpol	658.00		NIST Webbook
rinpol	659.00		NIST Webbook
rinpol	659.00		NIST Webbook
rinpol	658.00		NIST Webbook
rinpol	659.00		NIST Webbook
rinpol	660.00		NIST Webbook
rinpol	656.00		NIST Webbook
rinpol	659.00		NIST Webbook

rinpol	660.00		NIST Webbook
rinpol	661.00		NIST Webbook
rinpol	655.50		NIST Webbook
rinpol	656.50		NIST Webbook
rinpol	663.70		NIST Webbook
rinpol	665.60		NIST Webbook
rinpol	656.50		NIST Webbook
rinpol	658.00		NIST Webbook
rinpol	659.00		NIST Webbook
rinpol	655.00		NIST Webbook
rinpol	656.00		NIST Webbook
rinpol	661.00		NIST Webbook
rinpol	659.00		NIST Webbook
rinpol	664.00		NIST Webbook
rinpol	661.00		NIST Webbook
rinpol	663.30		NIST Webbook
rinpol	655.00		NIST Webbook
rinpol	663.70		NIST Webbook
rinpol	656.50		NIST Webbook
rinpol	665.60		NIST Webbook
rinpol	662.00		NIST Webbook
rinpol	655.60		NIST Webbook
tb	360.15 ± 1.00	K	NIST Webbook
tb	360.50 ± 0.50	K	NIST Webbook
tb	360.20 ± 0.50	K	NIST Webbook
tb	360.50 ± 0.60	K	NIST Webbook
tb	360.50 ± 1.00	K	NIST Webbook
tb	359.89 ± 0.30	K	NIST Webbook
tb	359.97 ± 0.30	K	NIST Webbook
tb	359.97 ± 0.30	K	NIST Webbook
tc	526.72	K	Joback Method
tf	131.70 ± 0.04	K	NIST Webbook
tf	131.65 ± 0.09	K	NIST Webbook
tf	131.66 ± 0.06	K	NIST Webbook
tf	131.70 ± 0.04	K	NIST Webbook
tf	131.66 ± 0.05	K	NIST Webbook
vc	0.403	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	243.44	J/molxK	526.72	Joback Method
cpg	180.32	J/molxK	355.80	Joback Method
cpg	191.94	J/molxK	384.29	Joback Method
cpg	203.10	J/molxK	412.77	Joback Method
cpg	213.82	J/molxK	441.26	Joback Method
cpg	224.10	J/molxK	469.74	Joback Method
cpg	233.97	J/molxK	498.23	Joback Method
dvisc	0.0002256	Paxs	355.80	Joback Method
dvisc	0.0078928	Paxs	151.89	Joback Method
dvisc	0.0025390	Paxs	185.88	Joback Method
dvisc	0.0011597	Paxs	219.86	Joback Method
dvisc	0.0006534	Paxs	253.84	Joback Method
dvisc	0.0004215	Paxs	287.83	Joback Method
dvisc	0.0002983	Paxs	321.82	Joback Method
hvapt	33.60	kJ/mol	348.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44355e+01
Coeff. B	-3.22439e+03
Coeff. C	-3.14360e+01
Temperature range (K), min.	259.34
Temperature range (K), max.	384.83

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	5.66732e+01
Coeff. B	-5.85380e+03
Coeff. C	-6.15233e+00
Coeff. D	3.23410e-06
Temperature range (K), min.	131.70
Temperature range (K), max.	534.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3769231&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.cheric.org/research/kdb/hcprop/showprop.php?cmpid=220
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/research/kdb/hcprop/showprop.php?cmpid=220

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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