

1-Hexene, 3-methyl-

Other names:	3-Methyl-1-hexene 3-methylhex-1-ene
Inchi:	InChI=1S/C7H14/c1-4-6-7(3)5-2/h5,7H,2,4,6H2,1,3H3
InchiKey:	RITONZMLZWYPHW-UHFFFAOYSA-N
Formula:	C7H14
SMILES:	C=CC(C)CCC
Mol. weight [g/mol]:	98.19
CAS:	3404-61-3

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	34.30	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	653.40		NIST Webbook
rinpol	644.80		NIST Webbook
rinpol	646.20		NIST Webbook
rinpol	685.00		NIST Webbook
rinpol	651.00		NIST Webbook
rinpol	651.00		NIST Webbook
rinpol	645.00		NIST Webbook
rinpol	645.50		NIST Webbook
rinpol	645.00		NIST Webbook
rinpol	646.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	643.00		NIST Webbook
rinpol	645.00		NIST Webbook
rinpol	647.00		NIST Webbook
rinpol	648.00		NIST Webbook
rinpol	651.00		NIST Webbook
rinpol	652.60		NIST Webbook
rinpol	643.00		NIST Webbook

rinpol	649.00			NIST Webbook
rinpol	643.90			NIST Webbook
rinpol	654.70			NIST Webbook
rinpol	645.00			NIST Webbook
rinpol	651.00			NIST Webbook
rinpol	645.00			NIST Webbook
rinpol	689.00			NIST Webbook
rinpol	646.00			NIST Webbook
rinpol	650.00			NIST Webbook
rinpol	647.00			NIST Webbook
rinpol	647.00			NIST Webbook
rinpol	695.00			NIST Webbook
rinpol	651.00			NIST Webbook
rinpol	650.20			NIST Webbook
rinpol	644.80			NIST Webbook
rinpol	645.00			NIST Webbook
rinpol	644.00			NIST Webbook
rinpol	643.10			NIST Webbook
rinpol	650.20			NIST Webbook
rinpol	645.00			NIST Webbook
rinpol	643.00			NIST Webbook
tb	360.00 ± 3.00		K	NIST Webbook
tb	357.02 ± 0.20		K	NIST Webbook
tb	357.19 ± 0.20		K	NIST Webbook
tb	357.15 ± 0.50		K	NIST Webbook
tb	357.05 ± 1.00		K	NIST Webbook
tb	357.20 ± 1.00		K	NIST Webbook
tb	357.09 ± 0.20		K	NIST Webbook
tc	526.72		K	Joback Method
tf	151.89		K	Joback Method
vc	0.403		m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.44	J/mol×K	526.72	Joback Method
cpg	180.32	J/mol×K	355.80	Joback Method
cpg	191.94	J/mol×K	384.29	Joback Method
cpg	203.10	J/mol×K	412.77	Joback Method
cpg	213.82	J/mol×K	441.26	Joback Method
cpg	224.10	J/mol×K	469.74	Joback Method

cpg	233.97	J/mol×K	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	33.40	kJ/mol	346.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42249e+01
Coeff. B	-3.03743e+03
Coeff. C	-4.08660e+01
Temperature range (K), min.	258.80
Temperature range (K), max.	381.64

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	8.62892e+01
Coeff. B	-6.92318e+03
Coeff. C	-1.07840e+01
Coeff. D	8.67407e-06
Temperature range (K), min.	145.00
Temperature range (K), max.	528.00

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C3404613&Units=SI>

The Yaws Handbook of Vapor

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Pressure:

KDB Vapor Pressure Data:

<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=219>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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=219
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/17-043-5/1-Hexene-3-methyl.pdf>

Generated by Cheméo on 2024-04-28 00:14:26.51955515 +0000 UTC m=+16552515.440132463.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.