2-Hexyne

Other names:	1-METHYL-2-PROPYLACETYLENE
	C3H7C«equiv»CCH3
	C3H7CÂ«equivÂ»CCH3
	Hex-2-yne
	Methyl(propyl)acetylene
Inchi:	InChI=1S/C6H10/c1-3-5-6-4-2/h3,5H2,1-2H3
InchiKey:	MELUCTCJOARQQG-UHFFFAOYSA-N
Formula:	C6H10
SMILES:	CC#CCCC
Mol. weight [g/mol]:	82.14
CAS:	764-35-2

Physical Properties

Property code	Value	Unit	Source
affp	806.10	kJ/mol	NIST Webbook
basg	781.10	kJ/mol	NIST Webbook
gf	202.44	kJ/mol	Joback Method
hf	107.70 ± 2.40	kJ/mol	NIST Webbook
hfus	14.42	kJ/mol	Joback Method
hvap	35.80	kJ/mol	NIST Webbook
hvap	35.90	kJ/mol	NIST Webbook
ie	9.97 ± 0.05	eV	NIST Webbook
ie	9.37 ± 0.01	eV	NIST Webbook
ie	9.37 ± 0.02	eV	NIST Webbook
ie	9.37 ± 0.05	eV	NIST Webbook
ie	9.37 ± 0.01	eV	NIST Webbook
log10ws	-2.13		Crippen Method
logp	1.810		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
rinpol	645.00		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	655.00		NIST Webbook
rinpol	655.00		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	644.00		NIST Webbook
rinpol	644.00		NIST Webbook

rinpol	638.00		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	642.20		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	639.00		NIST Webbook
rinpol	638.00		NIST Webbook
rinpol	638.00		NIST Webbook
rinpol	638.00		NIST Webbook
rinpol	645.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	644.00		NIST Webbook
rinpol	642.00		NIST Webbook
ripol	860.00		NIST Webbook
ripol	876.60		NIST Webbook
ripol	862.00		NIST Webbook
ripol	864.00		NIST Webbook
tb	357.00 ± 3.00	K	NIST Webbook
tb	356.95 ± 0.50	K	NIST Webbook
tb	359.15 ± 2.00	K	NIST Webbook
tb	356.65 ± 1.50	K	NIST Webbook
tb	357.00	K	NIST Webbook
tb	317.62 ± 0.30	K	NIST Webbook
tb	356.70 ± 1.00	K	NIST Webbook
tb	357.70	K	NIST Webbook
tb	84.45 ± 0.20	K	NIST Webbook
tb	357.00 ± 1.50	K	NIST Webbook
tb	357.00 ± 0.70	K	NIST Webbook
tb	357.65 ± 2.00	K	NIST Webbook
tb	356.65 ± 3.00	K	NIST Webbook
tb	356.65 ± 3.00	K	NIST Webbook
tb	357.67 ± 0.30	K	NIST Webbook
tb	356.55 ± 0.50	K	NIST Webbook
tb	357.28 ± 0.30	K	NIST Webbook
tb	357.34 ± 0.30	K	NIST Webbook
tb	357.00 ± 2.00	K	NIST Webbook
tb	357.70 ± 0.50	K	NIST Webbook
tc	534.57	K	Joback Method
tf	185.15 ± 1.50	K	NIST Webbook
tf	183.57 ± 0.30	K	NIST Webbook
vc	0.334	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.04	J/mol×K	345.68	Joback Method
cpg	147.09	J/mol×K	377.16	Joback Method
cpg	155.80	J/mol×K	408.64	Joback Method
cpg	164.19	J/mol×K	440.13	Joback Method
cpg	172.27	J/mol×K	471.61	Joback Method
cpg	180.04	J/mol×K	503.09	Joback Method
cpg	187.51	J/mol×K	534.57	Joback Method
hvapt	30.50	kJ/mol	303.50	NIST Webbook
hvapt	31.60	kJ/mol	275.50	NIST Webbook
pvap	12.75	kPa	303.15	Thermodynamics of isomeric hexynes +MTBE binary mixtures
pvap	2.61	kPa	273.15	Thermodynamics of isomeric hexynes +MTBE binary mixtures
pvap	4.63	kPa	283.15	Thermodynamics of isomeric hexynes +MTBE binary mixtures
pvap	7.84	kPa	293.15	Thermodynamics of isomeric hexynes +MTBE binary mixtures
pvap	10.05	kPa	298.15	Thermodynamics of isomeric hexynes +MTBE binary mixtures
pvap	1.39	kPa	263.15	Thermodynamics of isomeric hexynes +MTBE binary mixtures
pvap	19.99	kPa	313.15	Thermodynamics of isomeric hexynes +MTBE binary mixtures
pvap	30.32	kPa	323.15	Thermodynamics of isomeric hexynes +MTBE binary mixtures
pvap	44.66	kPa	333.15	Thermodynamics of isomeric hexynes +MTBE binary mixtures
pvap	64.09	kPa	343.15	Thermodynamics of isomeric hexynes +MTBE binary mixtures

pvap	1.37	kPa	263.15	Isothermal vapour liquid equilibria and excess molar enthalpies of hex-2-yne + methyl butyl ether and hex-3-yne + dibutyl ether mixtures	
pvap	2.56	kPa	273.15	Isothermal vapour liquid equilibria and excess molar enthalpies of hex-2-yne + methyl butyl ether and hex-3-yne + dibutyl ether mixtures	
pvap	4.53	kPa	283.15	Isothermal vapour liquid equilibria and excess molar enthalpies of hex-2-yne + methyl butyl ether and hex-3-yne + dibutyl ether mixtures	
pvap	7.66	kPa	293.15	Isothermal vapour liquid equilibria and excess molar enthalpies of hex-2-yne + methyl butyl ether and hex-3-yne + dibutyl ether mixtures	
pvap	9.80	kPa	298.15	Isothermal vapour liquid equilibria and excess molar enthalpies of hex-2-yne + methyl butyl ether and hex-3-yne + dibutyl ether mixtures	

pvap	12.43	kPa	303.15	Isothermal vapour liquid equilibria and excess molar enthalpies of hex-2-yne + methyl butyl ether and hex-3-yne + dibutyl ether mixtures
pvap	19.45	kPa	313.15	Isothermal vapour liquid equilibria and excess molar enthalpies of hex-2-yne + methyl butyl ether and hex-3-yne + dibutyl ether mixtures
pvap	29.46	kPa	323.15	Isothermal vapour liquid equilibria and excess molar enthalpies of hex-2-yne + methyl butyl ether and hex-3-yne + dibutyl ether mixtures
pvap	43.35	kPa	333.15	Isothermal vapour liquid equilibria and excess molar enthalpies of hex-2-yne + methyl butyl ether and hex-3-yne + dibutyl ether mixtures
pvap	62.15	kPa	343.15	Isothermal vapour liquid equilibria and excess molar enthalpies of hex-2-yne + methyl butyl ether and hex-3-yne + dibutyl ether mixtures

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38554e+01
Coeff. B	-2.83032e+03
Coeff. C	-5.12610e+01
Temperature range (K), min.	259.87
Temperature range (K), max.	382.53

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.73075e+01
Coeff. B	-7.03102e+03
Coeff. C	-1.08954e+01
Coeff. D	7.99421e-06
Temperature range (K), min.	183.65
Temperature range (K), max.	549.00

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Infinite dilution activity coefficients, specific retention volumes and solvation thermodynamics of hydrocarbons in C78H158 branched alkane solvent:	https://www.doi.org/10.1016/j.fluid.2006.07.015
Isothermal vapor liquid equilibria and excess enthalpies of binary mixtures of propyl ethanoate + 1-hexyne, +2-hexyne, +3-hexyne:	https://www.doi.org/10.1016/j.fluid.2010.10.022
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Isothermal vapour liquid equilibria and excess molar enthalpies of hex-2-yne + methyl butyl ether and hex-3-yne + dibutyl ether mixtures:	https://www.doi.org/10.1016/j.fluid.2007.09.002
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=408
KDB:	https://www.cheric.org/files/research/kdb/mol/mol408.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C764352&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermodynamics of isomeric hexynes +MTBE binary mixtures:	https://www.doi.org/10.1016/j.fluid.2006.08.007

Legend

affp:	Proton affinity
basg:	Gas basicity

cpg:	Ideal gas heat capacity
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
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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