## 1-Hexyne

Other names: BUTYLACETYLENE

Hex-1-yne Hexyne

N-BUTYLACETYLENE

NSC 9709

**Inchi:** InChl=1S/C6H10/c1-3-5-6-4-2/h1H,4-6H2,2H3

InchiKey: CGHIBGNXEGJPQZ-UHFFFAOYSA-N

Formula: C6H10
SMILES: C#CCCCC

**Mol. weight [g/mol]:** 82.14 **CAS:** 693-02-7

### **Physical Properties**

Value	Unit	Source
0.2490		KDB
799.80	kJ/mol	NIST Webbook
774.80	kJ/mol	NIST Webbook
222.71	kJ/mol	Joback Method
3889.86	kJ/mol	KDB
3670.205	kJ/mol	KDB
122.30 ± 1.20	kJ/mol	NIST Webbook
14.27	kJ/mol	Joback Method
28.81	kJ/mol	Joback Method
10.07 ± 0.01	eV	NIST Webbook
10.03 ± 0.05	eV	NIST Webbook
10.07 ± 0.02	eV	NIST Webbook
10.52 ± 0.05	eV	NIST Webbook
$9.95 \pm 0.05$	eV	NIST Webbook
-2.36		Estimated Solubility Method
-2.36		Aqueous Solubility Prediction Method
1.810		Crippen Method
86.800	ml/mol	McGowan Method
3690.00	kPa	KDB
610.00		NIST Webbook
586.00		NIST Webbook
	$0.2490$ $799.80$ $774.80$ $222.71$ $3889.86$ $3670.205$ $122.30 \pm 1.20$ $14.27$ $28.81$ $10.07 \pm 0.01$ $10.03 \pm 0.05$ $10.07 \pm 0.02$ $10.52 \pm 0.05$ $9.95 \pm 0.05$ $-2.36$ $1.810$ $86.800$ $3690.00$ $610.00$	0.2490         799.80       kJ/mol         774.80       kJ/mol         222.71       kJ/mol         3889.86       kJ/mol         3670.205       kJ/mol         122.30 ± 1.20       kJ/mol         14.27       kJ/mol         28.81       kJ/mol         10.07 ± 0.01       eV         10.03 ± 0.05       eV         10.07 ± 0.02       eV         10.52 ± 0.05       eV         9.95 ± 0.05       eV         -2.36       eV         1.810       86.800         86.800       ml/mol         3690.00       kPa         610.00

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rinpol	587.30		NIST Webbook
rinpol	612.00		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	584.00		
ripol	827.00		NIST Webbook
ripol	827.00		NIST Webbook
ripol	837.00		NIST Webbook
ripol	833.00		NIST Webbook
ripol	847.30		NIST Webbook
tb	323.15	K	NIST Webbook
tb	344.65 ± 1.00	K	NIST Webbook
tb	344.65 ± 0.70	K	NIST Webbook
tb	$344.50 \pm 0.30$	K	NIST Webbook
tb	344.52 ± 0.40	K	NIST Webbook
tb	344.65 ± 1.50	K	NIST Webbook
tb	343.65 ± 1.50	K	NIST Webbook
tb	344.40 ± 2.00	K	NIST Webbook
tb	344.65 ± 1.50	K	NIST Webbook
tb	344.55 ± 0.30	K	NIST Webbook
tb	344.00 ± 2.00	K	NIST Webbook
tb	343.35 ± 0.70	K	NIST Webbook
tb	345.05 ± 0.50	K	NIST Webbook
tb	344.65 ± 1.00	K	NIST Webbook
tb	344.48 ± 0.20	K	NIST Webbook
tb	344.53 ± 0.30	K	NIST Webbook
tb	344.00 ± 1.00	K	NIST Webbook
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tb	$344.15 \pm 1.50$	K	NIST Webbook
tb	344.15 ± 1.50	K	NIST Webbook
tb	343.45 ± 1.00	K	NIST Webbook
tb	344.70 ± 1.50	K	NIST Webbook
tb	$344.80 \pm 0.30$	K	NIST Webbook
tb	344.70 ± 1.00	K	NIST Webbook
tb	$344.80 \pm 0.40$	K	NIST Webbook
tb	344.70 ± 1.00	K	NIST Webbook
tb	$344.49 \pm 0.30$	K	NIST Webbook
tb	345.00 ± 1.00	K	NIST Webbook
tb	344.50	K	KDB
tb	343.65 ± 1.50	K	NIST Webbook
tb	343.65 ± 1.50	K	NIST Webbook
tb	344.15 ± 1.50	K	NIST Webbook
tb	344.15 ± 1.00	K	NIST Webbook
tb	344.15 ± 0.50	K	NIST Webbook
tb	345.15 ± 1.50	K	NIST Webbook
tb	$343.40 \pm 0.70$	K	NIST Webbook
tb	344.50	K	NIST Webbook
tc	529.00	K	KDB
tf	141.00	K	KDB
tf	141.15 ± 1.50	K	NIST Webbook
tf	141.06 ± 0.10	K	NIST Webbook
tf	140.75 ± 0.40	K	NIST Webbook
tf	141.18	K	Aqueous Solubility Prediction Method
VC	0.334	m3/kmol	KDB
ZC	0.2797890		KDB
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# **Temperature Dependent Properties**

Property code	Value	Unit	Temperature [K]	Source
cpg	186.81	J/mol×K	501.88	Joback Method
cpg	147.77	J/mol×K	355.98	Joback Method
cpg	138.91	J/mol×K	326.80	Joback Method
cpg	179.67	J/mol×K	472.70	Joback Method
cpg	172.20	J/mol×K	443.52	Joback Method
cpg	164.40	J/mol×K	414.34	Joback Method
cpg	156.26	J/mol×K	385.16	Joback Method
hvapt	33.50	kJ/mol	270.00	NIST Webbook
hvapt	34.20	kJ/mol	262.00	NIST Webbook

pvap         32.65         kPa         313.15         Thermodynamics of isomeric nexynes HMTBE binary mixtures           pvap         68.90         kPa         333.15         Thermodynamics of isomeric nexynes +MTBE binary mixtures           pvap         96.32         kPa         343.15         Thermodynamics of isomeric nexynes +MTBE binary mixtures           pvap         2.72         kPa         263.15         Thermodynamics of isomeric nexynes +MTBE binary mixtures           pvap         21.50         kPa         303.15         Thermodynamics of isomeric nexynes +MTBE binary mixtures           pvap         17.22         kPa         298.15         Thermodynamics of isomeric nexynes +MTBE binary mixtures           pvap         13.67         kPa         293.15         Thermodynamics of isomeric nexynes +MTBE binary mixtures           pvap         8.36         kPa         283.15         Thermodynamics of isomeric nexynes +MTBE binary mixtures           pvap         4.89         kPa         273.15         Thermodynamics of isomeric nexynes +MTBE binary mixtures           pvap         48.09         kPa         323.15         Thermodynamics of isomeric nexynes +MTBE binary mixtures           rfi         1.39600         298.15         KDB	hvapt	33.40	kJ/mol	328.00	NIST Webbook	
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rfi 1.39600 298.15 KDB	pvap	48.09	kPa	323.15	of isomeric hexynes +MTBE	
	rfi	1.39600		298.15	KDB	

## **Pressure Dependent Properties**

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	285.70	K	10.00	NIST Webbook

#### **Correlations**

Information	Value
Information	Value

Property code	pvap
Equation	In(Pvp) = A + B/(T + C)
Coeff. A	1.46089e+01
Coeff. B	-3.07754e+03
Coeff. C	-3.64370e+01
Temperature range (K), min.	251.33
Temperature range (K), max.	367.45

Information	Value

Property code	pvap
Equation	$ln(Pvp) = A + B/T + C*ln(T) + D*T^2$
Coeff. A	9.50798e+01
Coeff. B	-6.95750e+03
Coeff. C	-1.22828e+01
Coeff. D	1.25260e-05
Temperature range (K), min.	141.25
Temperature range (K), max.	516.20

#### Sources

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Determination of activity coefficients at https://www.doi.org/10.1016/j.fluid.2006.03.002
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ionic liquid choline

bis(trifluoromethylsulfonyl)imide:

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Legend

af: Acentric Factor affp: Proton affinity Gas basicity basg:

Ideal gas heat capacity cpg:

Standard Gibbs free energy of formation gf:

Heat of Combustion, Gross form hcg: hcn: Heat of Combustion, Net Form

hf: Enthalpy of formation at standard conditions hfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditions Enthalpy of vaporization at a given temperature hvapt:

ie: Ionization energy

Log10 of Water solubility in mol/l log10ws: Octanol/Water partition coefficient logp: mcvol: McGowan's characteristic volume

Critical Pressure pc: pvap: Vapor pressure rfi: Refractive Index

rinpol: Non-polar retention indices

ripol: Polar retention indices

tb: Normal Boiling Point Temperature tbrp: Boiling point at reduced pressure

tc: Critical Temperature tf: Normal melting (fusion) point

vc: Critical Volume

zc: Critical Compressibility

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