

1-Hexyne

Other names:	BUTYLACETYLENE Hex-1-yne Hexyne N-BUTYLACETYLENE NSC 9709
Inchi:	InChI=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

Property code	Value	Unit	Source
af	0.2490		KDB
affp	799.80	kJ/mol	NIST Webbook
basg	774.80	kJ/mol	NIST Webbook
gf	222.71	kJ/mol	Joback Method
hcg	3889.86	kJ/mol	KDB
hcn	3670.205	kJ/mol	KDB
hf	122.30 ± 1.20	kJ/mol	NIST Webbook
hfus	14.27	kJ/mol	Joback Method
hvap	28.81	kJ/mol	Joback Method
ie	10.07 ± 0.01	eV	NIST Webbook
ie	10.03 ± 0.05	eV	NIST Webbook
ie	10.07 ± 0.02	eV	NIST Webbook
ie	10.52 ± 0.05	eV	NIST Webbook
ie	9.95 ± 0.05	eV	NIST Webbook
log10ws	-2.36		Estimated Solubility Method
log10ws	-2.36		Aqueous Solubility Prediction Method
logp	1.810		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	3690.00	kPa	KDB
rinpol	610.00		NIST Webbook
rinpol	586.00		NIST Webbook

rinpol	586.00		NIST Webbook
rinpol	584.00		NIST Webbook
rinpol	588.00		NIST Webbook
rinpol	587.30		NIST Webbook
rinpol	587.00		NIST Webbook
rinpol	587.00		NIST Webbook
rinpol	584.00		NIST Webbook
rinpol	584.00		NIST Webbook
rinpol	584.00		NIST Webbook
rinpol	584.00		NIST Webbook
rinpol	583.00		NIST Webbook
rinpol	590.00		NIST Webbook
rinpol	588.20		NIST Webbook
rinpol	587.30		NIST Webbook
rinpol	586.00		NIST Webbook
rinpol	587.00		NIST Webbook
rinpol	587.00		NIST Webbook
rinpol	587.00		NIST Webbook
rinpol	587.30		NIST Webbook
rinpol	612.00		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	584.00		NIST Webbook
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 ± 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

tb	344.15 ± 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 ± 0.30	K	NIST Webbook
tb	344.70 ± 1.00	K	NIST Webbook
tb	344.80 ± 0.40	K	NIST Webbook
tb	344.70 ± 1.00	K	NIST Webbook
tb	344.49 ± 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 ± 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	m ³ /kmol	KDB
zc	0.2797890		KDB

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

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

Pressure Dependent Properties

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

tf: Normal melting (fusion) point
vc: Critical Volume
zc: Critical Compressibility

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