3-Hexyne

Other names:	C2H5C«equiv»CC2H5
	C2H5CÂ«equivÂ»CC2H5
	DIETHYLACETYLENE
	Hex-3-yne
Inchi:	InChI=1S/C6H10/c1-3-5-6-4-2/h3-4H2,1-2H3
InchiKey:	DQQNMIPXXNPGCV-UHFFFAOYSA-N
Formula:	C6H10
SMILES:	CCC#CCC
Mol. weight [g/mol]:	82.14
CAS:	928-49-4

Physical Properties

Property code	Value	Unit	Source
gf	202.44	kJ/mol	Joback Method
hf	105.40 ± 1.90	kJ/mol	NIST Webbook
hfus	14.42	kJ/mol	Joback Method
hvap	31.10	kJ/mol	Joback Method
ie	9.34 ± 0.05	eV	NIST Webbook
ie	9.32 ± 0.02	eV	NIST Webbook
ie	9.32 ± 0.01	eV	NIST Webbook
log10ws	-1.99		Aqueous Solubility Prediction Method
log10ws	-1.99		Estimated Solubility Method
logp	1.810		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
rinpol	619.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	620.00		NIST Webbook
rinpol	619.80		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	624.00		NIST Webbook
rinpol	627.00		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	622.00		NIST Webbook
rinpol	623.00		NIST Webbook

rinpol	624.00		NIST Webbook
rinpol	619.80		NIST Webbook
rinpol	621.60		NIST Webbook
rinpol	623.00		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	620.00		NIST Webbook
rinpol	620.00		NIST Webbook
rinpol	630.00		NIST Webbook
ripol	843.00		NIST Webbook
ripol	829.00		NIST Webbook
ripol	832.00		NIST Webbook
ripol	825.00		NIST Webbook
tb	354.58 ± 0.30	K	NIST Webbook
tb	354.61 ± 0.30	K	NIST Webbook
tb	353.65 ± 1.00	K	NIST Webbook
tb	353.65 ± 1.00	K	NIST Webbook
tb	354.35 ± 0.50	K	NIST Webbook
tb	354.45 ± 0.50	K	NIST Webbook
tb	354.15 ± 1.50	K	NIST Webbook
tb	353.90 ± 1.00	K	NIST Webbook
tb	354.95 ± 0.50	K	NIST Webbook
tb	354.60	K	NIST Webbook
tb	354.70	K	NIST Webbook
tb	354.45 ± 0.50	K	NIST Webbook
tb	353.00 ± 3.00	K	NIST Webbook
tc	534.57	K	Joback Method
tf	172.15 ± 1.50	K	NIST Webbook
tf	170.65 ± 0.30	K	NIST Webbook
tf	167.62 ± 0.10	K	NIST Webbook
tf	169.99 ± 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
pvap	3.00	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	1.61	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	5.29	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	8.91	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	11.38	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	14.39	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	22.40	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	33.77	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	49.44	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	70.52	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	1.41382e+01
Coeff. B	-3.03515e+03
Coeff. C	-3.55270e+01
Temperature range (K), min.	254.66
Temperature range (K), max.	379.39

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.15224e+01
Coeff. B	-5.47060e+03
Coeff. C	-5.42965e+00
Coeff. D	3.16370e-06
Temperature range (K), min.	170.05
Temperature range (K), max.	544.00

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
KDB:	https://www.cheric.org/files/research/kdb/mol/mol409.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=409
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C928494&Units=SI
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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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
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