1-Hexen-3-yne

Other names:	1-Hexene-3-yne
	C2H5C«equiv»CCH=CH2
	C2H5CÂ«equivÂ»CCH=CH2
	Ethylvinylacetylene
	Vinylethylacetylene
Inchi:	InChI=1S/C6H8/c1-3-5-6-4-2/h3H,1,4H2,2H3
InchiKey:	BYSRUWKGUGERFI-UHFFFAOYSA-N
Formula:	C6H8
SMILES:	C=CC#CCC
Mol. weight [g/mol]:	80.13
CAS:	13721-54-5

Physical Properties

Property code	Value	Unit	Source
gf	290.28	kJ/mol	Joback Method
hf	230.56	kJ/mol	Joback Method
hfus	13.14	kJ/mol	Joback Method
hvap	30.43	kJ/mol	Joback Method
ie	8.91 ± 0.01	eV	NIST Webbook
log10ws	-1.98		Crippen Method
logp	1.586		Crippen Method
mcvol	82.500	ml/mol	McGowan Method
pc	3945.61	kPa	Joback Method
tb	358.20	K	NIST Webbook
tb	356.90 ± 1.00	K	NIST Webbook
tb	356.65 ± 1.50	K	NIST Webbook
tc	535.51	K	Joback Method
tf	261.72	K	Joback Method
vc	0.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	125.24	J/mol×K	342.36	Joback Method

cpg	133.56	J/mol×K	374.55	Joback Method
cpg	141.53	J/mol×K	406.74	Joback Method
cpg	149.16	J/mol×K	438.94	Joback Method
cpg	156.47	J/mol×K	471.13	Joback Method
cpg	163.45	J/mol×K	503.32	Joback Method
cpg	170.13	J/mol×K	535.51	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52848e+01
Coeff. B	-3.38642e+03
Coeff. C	-4.07160e+01
Temperature range (K), min.	266.52
Temperature range (K), max.	380.27

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13721545&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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