

2-Hexen-4-yne

Other names:	Hex-2-en-4-yne
Inchi:	InChI=1S/C6H8/c1-3-5-6-4-2/h3,5H,1-2H3/b5-3+
InchiKey:	MASVKQBLNPTZME-HWKANZROSA-N
Formula:	C6H8
SMILES:	CC#CC=CC
Mol. weight [g/mol]:	80.13
CAS:	14092-20-7

Physical Properties

Property code	Value	Unit	Source
gf	282.66	kJ/mol	Joback Method
hf	222.35	kJ/mol	Joback Method
hfus	14.62	kJ/mol	Joback Method
hvap	31.06	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.586		Crippen Method
mcvol	82.500	ml/mol	McGowan Method
pc	3995.65	kPa	Joback Method
tb	359.40 ± 2.00	K	NIST Webbook
tc	549.54	K	Joback Method
tf	258.40	K	Joback Method
vc	0.314	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	123.85	J/mol×K	349.84	Joback Method
cpg	132.61	J/mol×K	383.12	Joback Method
cpg	140.94	J/mol×K	416.41	Joback Method
cpg	148.86	J/mol×K	449.69	Joback Method
cpg	156.38	J/mol×K	482.97	Joback Method
cpg	163.53	J/mol×K	516.26	Joback Method
cpg	170.33	J/mol×K	549.54	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.55621e+01
Coeff. B	-3.47694e+03
Coeff. C	-4.16890e+01
Temperature range (K), min.	269.32
Temperature range (K), max.	380.88

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	https://webbook.nist.gov/cgi/cbook.cgi?ID=C14092207&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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