

3-Hexen-1-yne

Other names:	3-Hex-3-en-1-yne
Inchi:	InChI=1S/C6H8/c1-3-5-6-4-2/h1,5-6H,4H2,2H3/b6-5+
InchiKey:	CLFYLSQRWCJAY-AATRIKPKSA-N
Formula:	C6H8
SMILES:	C#CC=CCC
Mol. weight [g/mol]:	80.13
CAS:	2806-56-6

Physical Properties

Property code	Value	Unit	Source
gf	302.93	kJ/mol	Joback Method
hf	241.95	kJ/mol	Joback Method
hfus	14.47	kJ/mol	Joback Method
hvap	28.77	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.586		Crippen Method
mcvol	82.500	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
tb	346.00 ± 3.00	K	NIST Webbook
tc	516.12	K	Joback Method
tf	199.27	K	Joback Method
vc	0.314	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	125.17	J/mol×K	330.96	Joback Method
cpg	133.83	J/mol×K	361.82	Joback Method
cpg	142.01	J/mol×K	392.68	Joback Method
cpg	149.75	J/mol×K	423.54	Joback Method
cpg	157.07	J/mol×K	454.40	Joback Method
cpg	163.99	J/mol×K	485.26	Joback Method
cpg	170.53	J/mol×K	516.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2806566&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/44-680-8/3-Hexen-1-yne.pdf>

Generated by Cheméo on 2025-12-19 15:52:02.855769764 +0000 UTC m=+5907720.385810418.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.