

4-Nonen-2-yne, (Z)-

Other names:	Non-2-yn-4-ene, (Z)-
Inchi:	InChI=1S/C9H14/c1-3-5-7-9-8-6-4-2/h8-9H,3,5,7H2,1-2H3/b9-8-
InchiKey:	AIDMRHRNBMILQM-HJWRWDBZSA-N
Formula:	C9H14
SMILES:	CC#CC=CCCC
Mol. weight [g/mol]:	122.21
CAS:	53497-78-2

Physical Properties

Property code	Value	Unit	Source
gf	307.92	kJ/mol	Joback Method
hf	160.43	kJ/mol	Joback Method
hfus	22.39	kJ/mol	Joback Method
hvap	37.74	kJ/mol	Joback Method
ie	8.46 ± 0.01	eV	NIST Webbook
log10ws	-3.24		Crippen Method
logp	2.756		Crippen Method
mcvol	124.770	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
tb	418.48	K	Joback Method
tc	614.03	K	Joback Method
tf	292.21	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.02	J/molxK	418.48	Joback Method
cpg	245.08	J/molxK	451.07	Joback Method
cpg	257.51	J/molxK	483.66	Joback Method
cpg	269.36	J/molxK	516.26	Joback Method
cpg	280.63	J/molxK	548.85	Joback Method
cpg	291.36	J/molxK	581.44	Joback Method
cpg	301.57	J/molxK	614.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53497782&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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