2-Methyl-1-hepten-3-yne

Other names:	n-C3H7C«equiv»CC(CH3)=CH2
	1-Hepten-3-yne, 2-methyl-
	2-Methyl-hept-1-en-3-yne
	2-Methyl-1-heptene-3-yne
Inchi:	InChI=1S/C8H12/c1-4-5-6-7-8(2)3/h2,4-5H2,1,3H3
InchiKey:	UOOFRLPCQNNECP-UHFFFAOYSA-N
Formula:	C8H12
SMILES:	C=C(C)C#CCCC
Mol. weight [g/mol]:	108.18
CAS:	17669-40-8

Physical Properties

Property code	Value	Unit	Source
gf	298.57	kJ/mol	Joback Method
hf	179.49	kJ/mol	Joback Method
hfus	17.01	kJ/mol	Joback Method
hvap	34.96	kJ/mol	Joback Method
ie	8.62 ± 0.01	eV	NIST Webbook
log10ws	-2.82		Crippen Method
logp	2.366		Crippen Method
mcvol	110.680	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
tb	388.00	K	Joback Method
tc	583.37	K	Joback Method
tf	270.30	K	Joback Method
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.88	J/mol×K	388.00	Joback Method
cpg	205.47	J/mol×K	420.56	Joback Method
cpg	216.54	J/mol×K	453.12	Joback Method
cpg	227.12	J/mol×K	485.69	Joback Method

cpg	237.22	J/mol×K	518.25	Joback Method
cpg	246.87	J/mol×K	550.81	Joback Method
cpg	256.07	J/mol×K	583.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17669408&Units=SI
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

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