1-Penten-3-yne, 2-methyl-

Other names: CH3C«equiv»CC(CH3)=CH2
2-Methyl-1-pentene-3-yne
Inchi: InChI=1S/C6H8/c1-4-5-6(2)3/h2H2,1,3H3
InchiKey: KGIABMDFILVKGN-UHFFFAOYSA-N
Formula: C6H8
SMILES: C=C(C)C#CC
Mol. weight [g/mol]: 80.13
CAS: 926-55-6

Physical Properties

Property code	Value	Unit	Source
gf	281.73	kJ/mol	Joback Method
hf	220.77	kJ/mol	Joback Method
hfus	11.83	kJ/mol	Joback Method
hvap	30.51	kJ/mol	Joback Method
ie	8.72 ± 0.01	eV	NIST Webbook
log10ws	-1.98		Crippen Method
logp	1.586		Crippen Method
mcvol	82.500	ml/mol	McGowan Method
pc	3970.51	kPa	Joback Method
tb	355.50 ± 0.50	K	NIST Webbook
tc	539.62	K	Joback Method
tf	247.76	K	Joback Method
vc	0.316	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	125.29	J/mol×K	342.24	Joback Method
cpg	133.76	J/mol×K	375.14	Joback Method
cpg	141.86	J/mol×K	408.03	Joback Method
cpg	149.61	J/mol×K	440.93	Joback Method
cpg	157.01	J/mol×K	473.83	Joback Method
cpg	164.08	J/mol×K	506.73	Joback Method

cpg	170.84	J/mol×K	539.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C926556&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