HC«equiv»CCOCH2CH2CH3

Other names:	1-Hexyn-3-one
	Ethynyl propyl ketone
	Hex-1-yn-3-one
	1-Hexyne-3-one
Inchi:	InChI=1S/C6H8O/c1-3-5-6(7)4-2/h2H,3,5H2,1H3
InchiKey:	KSJAIMUFADDAOP-UHFFFAOYSA-N
Formula:	C6H8O
SMILES:	C#CC(=O)CCC
Mol. weight [g/mol]:	96.13
CAS:	689-00-9

Physical Properties

Property code	Value	Unit	Source
gf	93.79	kJ/mol	Joback Method
hf	12.15	kJ/mol	Joback Method
hfus	15.87	kJ/mol	Joback Method
hvap	35.55	kJ/mol	Joback Method
ie	10.22 ± 0.04	eV	NIST Webbook
ie	9.94	eV	NIST Webbook
log10ws	-1.41		Crippen Method
logp	0.989		Crippen Method
mcvol	88.370	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
tb	380.67	K	Joback Method
tc	571.29	K	Joback Method
tf	254.28	K	Joback Method
vc	0.340	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	153.89	J/mol×K	380.67	Joback Method
cpg	162.24	J/mol×K	412.44	Joback Method
cpg	170.20	J/mol×K	444.21	Joback Method

cpg	177.78	J/mol×K	475.98	Joback Method
cpg	184.99	J/mol×K	507.75	Joback Method
cpg	191.86	J/mol×K	539.52	Joback Method
cpg	198.39	J/mol×K	571.29	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	338.70	K	13.30	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C689009&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume