Hex-2-yn-4-one, 2-methyl-

Other names: 2-Methyl-4-hexyne-3-one
Inchi: InChI=1S/C7H10O/c1-4-5-7(8)6(2)3/h6H,1-3H3
InchiKey: XYKVPEZERYZDJY-UHFFFAOYSA-N
Formula: C7H10O
SMILES: CC#CC(=O)C(C)C
Mol. weight [g/mol]: 110.15
CAS: 52066-33-8

Physical Properties

Property code	Value	Unit	Source
gf	79.50	kJ/mol	Joback Method
hf	-33.37	kJ/mol	Joback Method
hfus	15.08	kJ/mol	Joback Method
hvap	39.69	kJ/mol	Joback Method
ie	9.50	eV	NIST Webbook
log10ws	-1.59		Crippen Method
logp	1.235		Crippen Method
mcvol	102.460	ml/mol	McGowan Method
pc	3633.35	kPa	Joback Method
tb	421.99	K	Joback Method
tc	628.86	K	Joback Method
tf	309.68	K	Joback Method
vc	0.390	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.19	J/mol×K	421.99	Joback Method
cpg	198.60	J/mol×K	456.47	Joback Method
cpg	208.55	J/mol×K	490.95	Joback Method
cpg	218.06	J/mol×K	525.43	Joback Method
cpg	227.13	J/mol×K	559.91	Joback Method
cpg	235.77	J/mol×K	594.39	Joback Method
cpg	244.00	J/mol×K	628.86	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52066338&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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