Hex-4-yn-3-one, 2,2-dimethyl-

Other names: 2,2-Dimethyl-4-hexyne-3-one
Inchi: InChI=1S/C8H12O/c1-5-6-7(9)8(2,3)4/h1-4H3
InchiKey: UDGLAQDRKQGIKX-UHFFFAOYSA-N
Formula: C8H12O
SMILES: CC#CC(=O)C(C)(C)C
Mol. weight [g/mol]: 124.18
CAS: 71932-99-5

Physical Properties

Property code	Value	Unit	Source
gf	93.20	kJ/mol	Joback Method
hf	-57.48	kJ/mol	Joback Method
hfus	13.78	kJ/mol	Joback Method
hvap	41.00	kJ/mol	Joback Method
ie	9.42	eV	NIST Webbook
log10ws	-2.00		Crippen Method
logp	1.625		Crippen Method
mcvol	116.550	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
tb	442.08	K	Joback Method
tc	655.54	K	Joback Method
tf	338.37	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.32	J/mol×K	442.08	Joback Method
cpg	242.04	J/mol×K	477.66	Joback Method
cpg	254.01	J/mol×K	513.23	Joback Method
cpg	265.28	J/mol×K	548.81	Joback Method
cpg	275.87	J/mol×K	584.39	Joback Method
cpg	285.83	J/mol×K	619.96	Joback Method
cpg	295.19	J/mol×K	655.54	Joback Method

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=C71932995&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume