3-Octyn-2-one

Other names:	Butyl(acetyl)acetylene
	Acetylbutylacetylene
	Oct-3-yn-2-one
	3-Octyne-2-one
Inchi:	InChI=1S/C8H12O/c1-3-4-5-6-7-8(2)9/h3-5H2,1-2H3
InchiKey:	VJKHTMGYHCBXHV-UHFFFAOYSA-N
Formula:	C8H12O
SMILES:	CCCCC#CC(C)=O
Mol. weight [g/mol]:	124.18
CAS:	1119-58-0

Physical Properties

Property code	Value	Unit	Source
gf	90.36	kJ/mol	Joback Method
hf	-48.73	kJ/mol	Joback Method
hfus	21.20	kJ/mol	Joback Method
hvap	42.30	kJ/mol	Joback Method
ie	9.64	eV	NIST Webbook
log10ws	-2.25		Crippen Method
logp	1.769		Crippen Method
mcvol	116.550	ml/mol	McGowan Method
pc	3217.33	kPa	Joback Method
tb	445.31	K	Joback Method
tc	645.05	K	Joback Method
tf	335.95	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.66	J/mol×K	445.31	Joback Method
cpg	238.08	J/mol×K	478.60	Joback Method
cpg	249.00	J/mol×K	511.89	Joback Method
cpg	259.44	J/mol×K	545.18	Joback Method

cpg	269.40	J/mol×K	578.47	Joback Method
cpg	278.91	J/mol×K	611.76	Joback Method
cpg	287.97	J/mol×K	645.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1119580&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

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