2-Pentyn-4-one

Other names:	3-Pentyn-2-one
	Pent-3-yn-2-one
	3-Pentyne-2-one
Inchi:	InChI=1S/C5H6O/c1-3-4-5(2)6/h1-2H3
InchiKey:	DZOOXMGZVWHNAS-UHFFFAOYSA-N
Formula:	C5H6O
SMILES:	CC#CC(C)=O
Mol. weight [g/mol]:	82.10
CAS:	7299-55-0

Physical Properties

Property code	Value	Unit	Source
gf	65.10	kJ/mol	Joback Method
hf	13.19	kJ/mol	Joback Method
hfus	13.43	kJ/mol	Joback Method
hvap	35.62	kJ/mol	Joback Method
ie	9.76	eV	NIST Webbook
log10ws	-0.99		Crippen Method
logp	0.599		Crippen Method
mcvol	74.280	ml/mol	McGowan Method
pc	4596.38	kPa	Joback Method
tb	376.67	K	Joback Method
tc	582.35	K	Joback Method
tf	302.14	K	Joback Method
vc	0.283	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	118.14	J/mol×K	376.67	Joback Method
cpg	125.04	J/mol×K	410.95	Joback Method
cpg	131.67	J/mol×K	445.23	Joback Method
cpg	138.04	J/mol×K	479.51	Joback Method
cpg	144.14	J/mol×K	513.79	Joback Method

cpg	149.99	J/mol×K	548.07	Joback Method
cpg	155.59	J/mol×K	582.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7299550&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