Pent-1-yn-3-one

Other names: 1-Pentyne-3-one
Inchi: InChI=1S/C5H6O/c1-3-5(6)4-2/h1H,4H2,2H3
InchiKey: GBCOTHPVQOTZKQ-UHFFFAOYSA-N
Formula: C5H6O
SMILES: C#CC(=O)CC
Mol. weight [g/mol]: 82.10
CAS: 16469-62-8

Physical Properties

Property code	Value	Unit	Source
gf	85.37	kJ/mol	Joback Method
hf	32.79	kJ/mol	Joback Method
hfus	13.28	kJ/mol	Joback Method
hvap	33.33	kJ/mol	Joback Method
ie	10.03	eV	NIST Webbook
log10ws	-0.99		Crippen Method
logp	0.599		Crippen Method
mcvol	74.280	ml/mol	McGowan Method
pc	4522.49	kPa	Joback Method
tb	357.79	K	Joback Method
tc	549.33	K	Joback Method
tf	243.01	K	Joback Method
vc	0.283	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	120.97	J/mol×K	357.79	Joback Method
cpg	127.75	J/mol×K	389.71	Joback Method
cpg	134.22	J/mol×K	421.64	Joback Method
cpg	140.37	J/mol×K	453.56	Joback Method
cpg	146.22	J/mol×K	485.48	Joback Method
cpg	151.79	J/mol×K	517.41	Joback Method
cpg	157.08	J/mol×K	549.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16469628&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