Pent-1-yn-3-yl

Other names: Pent-1-yn-3-yl radical
Inchi: InChI=1S/C5H7/c1-3-5-4-2/h1,5H,4H2,2H3
InchiKey: PHBDUZYYMFTIDN-UHFFFAOYSA-N
Formula: C5H7
SMILES: C#C[CH]CC
Mol. weight [g/mol]: 67.11
CAS: 115236-80-1

Physical Properties

Property code	Value	Unit	Source
gf	264.23	kJ/mol	Joback Method
hf	195.90	kJ/mol	Joback Method
hfus	9.84	kJ/mol	Joback Method
hvap	26.05	kJ/mol	Joback Method
ie	7.60	eV	NIST Webbook
log10ws	-1.32		Crippen Method
logp	1.234		Crippen Method
mcvol	70.560	ml/mol	McGowan Method
pc	4456.32	kPa	Joback Method
tb	302.78	K	Joback Method
tc	478.11	K	Joback Method
tf	194.45	K	Joback Method
vc	0.263	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	102.74	J/mol×K	302.78	Joback Method
cpg	110.29	J/mol×K	332.00	Joback Method
cpg	117.35	J/mol×K	361.22	Joback Method
cpg	123.96	J/mol×K	390.45	Joback Method
cpg	130.15	J/mol×K	419.67	Joback Method
cpg	135.93	J/mol×K	448.89	Joback Method
cpg	141.34	J/mol×K	478.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C115236801&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