

Pent-1-en-4-yn-3-yl radical

Inchi:	InChI=1S/C5H5/c1-3-5-4-2/h1,4-5H,2H2
InchiKey:	MOHCYMPYDWGDHY-UHFFFAOYSA-N
Formula:	C5H5
SMILES:	C#C[CH]C=C
Mol. weight [g/mol]:	65.09
CAS:	78596-31-3

Physical Properties

Property code	Value	Unit	Source
gf	352.07	kJ/mol	Joback Method
hf	321.33	kJ/mol	Joback Method
hfus	8.56	kJ/mol	Joback Method
hvap	25.38	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	1.010		Crippen Method
mcvol	66.260	ml/mol	McGowan Method
pc	4717.12	kPa	Joback Method
tb	299.46	K	Joback Method
tc	478.63	K	Joback Method
tf	192.69	K	Joback Method
vc	0.243	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	91.28	J/mol×K	299.46	Joback Method
cpg	98.17	J/mol×K	329.32	Joback Method
cpg	104.54	J/mol×K	359.18	Joback Method
cpg	110.43	J/mol×K	389.04	Joback Method
cpg	115.87	J/mol×K	418.91	Joback Method
cpg	120.89	J/mol×K	448.77	Joback Method
cpg	125.52	J/mol×K	478.63	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78596313&Units=SI

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
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

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