Benzene, 1-ethynyl-4-methoxy-

Other names:	4-Methoxyphenylacetylene
	4-CH3O-C6H4-CCH
Inchi:	InChI=1S/C9H8O/c1-3-8-4-6-9(10-2)7-5-8/h1,4-7H,2H3
InchiKey:	KBIAVTUACPKPFJ-UHFFFAOYSA-N
Formula:	C9H8O
SMILES:	C#Cc1ccc(OC)cc1
Mol. weight [g/mol]:	132.16
CAS:	768-60-5

Physical Properties

Property code	Value	Unit	Source
affp	886.40	kJ/mol	NIST Webbook
basg	855.70	kJ/mol	NIST Webbook
gf	245.75	kJ/mol	Joback Method
hf	155.65	kJ/mol	Joback Method
hfus	16.88	kJ/mol	Joback Method
hvap	40.83	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	1.676		Crippen Method
mcvol	111.180	ml/mol	McGowan Method
pc	3740.80	kPa	Joback Method
tb	449.52	K	Joback Method
tc	672.74	K	Joback Method
tf	299.33	K	Joback Method
vc	0.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.43	J/mol×K	449.52	Joback Method
cpg	220.89	J/mol×K	486.72	Joback Method
cpg	231.72	J/mol×K	523.93	Joback Method
cpg	241.94	J/mol×K	561.13	Joback Method
cpg	251.57	J/mol×K	598.33	Joback Method

cpg	260.63	J/mol×K	635.53	Joback Method
cpg	269.13	J/mol×K	672.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C768605&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

affp:	Proton affinity
basg:	Gas basicity
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