Benzene, 1-ethynyl-4-methyl-

Other names:	Toluene, p-ethynyl-
	p-Ethynyltoluene
	p-Methylphenylacetylene
	p-Tolylacetylene
	4-Methylphenylacetylene
	4-Ethynyltoluene
	4-Methylethynylbenzene
	1-ethynyl-4-methylbenzene
Inchi:	InChI=1S/C9H8/c1-3-9-6-4-8(2)5-7-9/h1,4-7H,2H3
InchiKey:	KSZVOXHGCKKOLL-UHFFFAOYSA-N
Formula:	C9H8
SMILES:	C#Cc1ccc(C)cc1
Mol. weight [g/mol]:	116.16
CAS:	766-97-2

Physical Properties

Property code	Value	Unit	Source
affp	853.20	kJ/mol	NIST Webbook
basg	822.50	kJ/mol	NIST Webbook
gf	350.75	kJ/mol	Joback Method
hf	287.87	kJ/mol	Joback Method
hfus	15.69	kJ/mol	Joback Method
hvap	38.42	kJ/mol	Joback Method
ie	8.43	eV	NIST Webbook
ie	8.48 ± 0.02	eV	NIST Webbook
log10ws	-2.65		Crippen Method
logp	1.976		Crippen Method
mcvol	105.310	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
rinpol	165.70		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	151.80		NIST Webbook
rinpol	169.80		NIST Webbook
ripol	1454.30		NIST Webbook
tb	442.20	K	NIST Webbook
tc	652.10	K	Joback Method
tf	277.10	K	Joback Method

vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.73	J/mol×K	427.10	Joback Method
cpg	199.55	J/mol×K	464.60	Joback Method
cpg	210.63	J/mol×K	502.10	Joback Method
cpg	221.00	J/mol×K	539.60	Joback Method
cpg	230.69	J/mol×K	577.10	Joback Method
cpg	239.74	J/mol×K	614.60	Joback Method
cpg	248.19	J/mol×K	652.10	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C766972&Units=SI

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure

rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume