Benzene, 1-ethynyl-4-fluoro-

Other names:	(p-Fluorophenyl)acetylene
	4-FC6H4CCH
	4-fluorophenylacetylene
Inchi:	InChI=1S/C8H5F/c1-2-7-3-5-8(9)6-4-7/h1,3-6H
InchiKey:	QXSWHQGIEKUBAS-UHFFFAOYSA-N
Formula:	C8H5F
SMILES:	C#Cc1ccc(F)cc1
Mol. weight [g/mol]:	120.12
CAS:	766-98-3

Physical Properties

Property code	Value	Unit	Source
affp	827.40	kJ/mol	NIST Webbook
basg	796.70	kJ/mol	NIST Webbook
gf	147.52	kJ/mol	Joback Method
hf	112.40	kJ/mol	Joback Method
hfus	16.18	kJ/mol	Joback Method
hvap	35.38	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	1.807		Crippen Method
mcvol	92.990	ml/mol	McGowan Method
pc	4072.51	kPa	Joback Method
tb	403.49	K	Joback Method
tc	618.34	K	Joback Method
tf	266.42	K	Joback Method
vc	0.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	159.08	J/mol×K	403.49	Joback Method
cpg	168.90	J/mol×K	439.30	Joback Method
cpg	178.09	J/mol×K	475.11	Joback Method
cpg	186.69	J/mol×K	510.91	Joback Method

cpg	194.72	J/mol×K	546.72	Joback Method
cpg	202.21	J/mol×K	582.53	Joback Method
cpg	209.19	J/mol×K	618.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C766983&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