Benzene, 1-chloro-4-ethynyl-

Other names: (p-Chlorophenyl)acetylene
(4-Chlorophenyl)acetylene
p-Ethynylchlorobenzene
1-Chloro-4-ethynylbenzene
Inchi: InChI=1S/C8H5Cl/c1-2-7-3-5-8(9)6-4-7/h1,3-6H
InchiKey: LFZJRTMTKGYJRS-UHFFFAOYSA-N
Formula: C8H5Cl
SMILES: C#Cc1ccc(Cl)cc1
Mol. weight [g/mol]: 136.58
CAS: 873-73-4

Physical Properties

Property code	Value	Unit	Source
affp	832.40	kJ/mol	NIST Webbook
basg	801.70	kJ/mol	NIST Webbook
gf	330.40	kJ/mol	Joback Method
hf	292.77	kJ/mol	Joback Method
hfus	17.30	kJ/mol	Joback Method
hvap	40.58	kJ/mol	Joback Method
ie	8.75	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
log10ws	-2.86		Crippen Method
logp	2.321		Crippen Method
mcvol	103.460	ml/mol	McGowan Method
pc	4114.41	kPa	Joback Method
tb	441.65	K	Joback Method
tc	677.32	K	Joback Method
tf	295.75	K	Joback Method
vc	0.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.63	J/mol×K	441.65	Joback Method

cpg	183.38	J/mol×K	480.93	Joback Method
cpg	192.42	J/mol×K	520.21	Joback Method
cpg	200.79	J/mol×K	559.49	Joback Method
cpg	208.54	J/mol×K	598.77	Joback Method
cpg	215.69	J/mol×K	638.04	Joback Method
cpg	222.30	J/mol×K	677.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C873734&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
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