Benzene,(chloroethynyl)-

Other names: 2-Chloro-1-phenylacetylene
Inchi: InChI=1S/C8H5Cl/c9-7-6-8-4-2-1-3-5-8/h1-5H
InchiKey: GDWZLADUGAKASM-UHFFFAOYSA-N
Formula: C8H5Cl
SMILES: ClC#Cc1ccccc1
Mol. weight [g/mol]: 136.58
CAS: 1483-82-5

Physical Properties

Property code	Value	Unit	Source
gf	319.76	kJ/mol	Joback Method
hf	284.64	kJ/mol	Joback Method
hfus	17.84	kJ/mol	Joback Method
hvap	42.22	kJ/mol	Joback Method
ie	8.70	eV	NIST Webbook
log10ws	-2.82		Crippen Method
logp	2.234		Crippen Method
mcvol	103.460	ml/mol	McGowan Method
pc	4260.71	kPa	Joback Method
tb	455.55	K	Joback Method
tc	704.66	K	Joback Method
tf	342.36	K	Joback Method
vc	0.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.28	J/mol×K	455.55	Joback Method
cpg	181.86	J/mol×K	497.07	Joback Method
cpg	191.67	J/mol×K	538.59	Joback Method
cpg	200.75	J/mol×K	580.10	Joback Method
cpg	209.13	J/mol×K	621.62	Joback Method
cpg	216.85	J/mol×K	663.14	Joback Method
cpg	223.97	J/mol×K	704.66	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=C1483825&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
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