Benzene, 1-propynyl-

Other names:	Methylphenylacetylene
	Phenylmethylacetylene
	1-Methyl-2-phenylacetylene
	1-Phenyl-1-propyne
	1-Phenylpropyne
	1-Propynylbenzene
	1-Phenylpropyne-1
	Methylphenylethyne
	Propyne, 1-phenyl-
	prop-1-ynylbenzene
Inchi:	InChI=1S/C9H8/c1-2-6-9-7-4-3-5-8-9/h3-5,7-8H,1H3
InchiKey:	GHUURDQYRGVEHX-UHFFFAOYSA-N
Formula:	C9H8
SMILES:	CC#Cc1ccccc1
Mol. weight [g/mol]:	116.16
CAS:	673-32-5

Physical Properties

Property code	Value	Unit	Source
gf	340.11	kJ/mol	Joback Method
hf	268.20 ± 2.20	kJ/mol	NIST Webbook
hfus	16.23	kJ/mol	Joback Method
hvap	40.06	kJ/mol	Joback Method
ie	8.41 ± 0.02	eV	NIST Webbook
ie	8.49	eV	NIST Webbook
ie	8.42 ± 0.08	eV	NIST Webbook
log10ws	-2.59		Crippen Method
logp	2.058		Crippen Method
mcvol	105.310	ml/mol	McGowan Method
pc	3950.57	kPa	Joback Method
rinpol	1058.00		NIST Webbook
rinpol	167.60		NIST Webbook
rinpol	149.70		NIST Webbook
rinpol	153.30		NIST Webbook
rinpol	167.60		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	149.70		NIST Webbook

rinpol	1035.00		NIST Webbook
tb	456.00	K	NIST Webbook
tb	458.20	K	NIST Webbook
tc	679.04	K	Joback Method
tf	323.71	K	Joback Method
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.11	J/mol×K	441.00	Joback Method
cpg	198.85	J/mol×K	480.67	Joback Method
cpg	210.76	J/mol×K	520.35	Joback Method
cpg	221.90	J/mol×K	560.02	Joback Method
cpg	232.29	J/mol×K	599.70	Joback Method
cpg	241.97	J/mol×K	639.37	Joback Method
cpg	250.99	J/mol×K	679.04	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	363.00	K	2.70	NIST Webbook

Sources

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=C673325&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume