Benzene, 1-butynyl-

Other names:	1-Butyne, 1-phenyl-
	1-Butynylbenzene
	Ethylphenylacetylene
	1-Ethyl-2-phenylacetylene
	1-Phenyl-1-butyne
	Phenylethylacetylene
Inchi:	InChI=1S/C10H10/c1-2-3-7-10-8-5-4-6-9-10/h4-6,8-9H,2H2,1H3
InchiKey:	FFFMSANAQQVUJA-UHFFFAOYSA-N
Formula:	C10H10
SMILES:	CCC#Cc1ccccc1
Mol. weight [g/mol]:	130.19
CAS:	622-76-4

Physical Properties

Property code	Value	Unit	Source
gf	348.53	kJ/mol	Joback Method
hf	248.60 ± 1.00	kJ/mol	NIST Webbook
hfus	18.82	kJ/mol	Joback Method
hvap	42.28	kJ/mol	Joback Method
ie	8.37 ± 0.08	eV	NIST Webbook
ie	8.30	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
ie	8.33 ± 0.02	eV	NIST Webbook
log10ws	-3.01		Crippen Method
logp	2.448		Crippen Method
mcvol	119.400	ml/mol	McGowan Method
pc	3513.74	kPa	Joback Method
rinpol	1129.00		NIST Webbook
rinpol	191.40		NIST Webbook
rinpol	191.40		NIST Webbook
rinpol	1118.00		NIST Webbook
rinpol	1129.00		NIST Webbook
tb	475.20	K	NIST Webbook
tb	473.00 ± 5.00	K	NIST Webbook
tb	463.60 ± 3.00	K	NIST Webbook
tc	698.04	K	Joback Method
tf	334.98	K	Joback Method

vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.20	J/mol×K	463.88	Joback Method
cpg	240.25	J/mol×K	502.91	Joback Method
cpg	253.41	J/mol×K	541.93	Joback Method
cpg	265.73	J/mol×K	580.96	Joback Method
cpg	277.24	J/mol×K	619.98	Joback Method
cpg	287.99	J/mol×K	659.01	Joback Method
cpg	298.02	J/mol×K	698.04	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	347.20	K	0.50	NIST Webbook
tbrp	353.00	K	1.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C622764&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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