Benzene, cyclopropyl-

Other names:	Cyclopropane, phenyl-
	Cyclopropylbenzene
	Phenylcyclopropane
	1-Phenylcyclopropane
Inchi:	InChI=1S/C9H10/c1-2-4-8(5-3-1)9-6-7-9/h1-5,9H,6-7H2
InchiKey:	VFSFCYAQBIPUSL-UHFFFAOYSA-N
Formula:	C9H10
SMILES:	c1ccc(C2CC2)cc1
Mol. weight [g/mol]:	118.18
CAS:	873-49-4

Physical Properties

Property code	Value	Unit	Source
affp	834.90	kJ/mol	NIST Webbook
affp	832.20	kJ/mol	NIST Webbook
basg	802.40	kJ/mol	NIST Webbook
basg	802.50	kJ/mol	NIST Webbook
chl	-5071.00 ± 0.80	kJ/mol	NIST Webbook
chl	-5076.40	kJ/mol	NIST Webbook
gf	198.06	kJ/mol	Joback Method
hf	150.70 ± 1.00	kJ/mol	NIST Webbook
hf	150.40 ± 0.80	kJ/mol	NIST Webbook
hfl	100.20 ± 0.80	kJ/mol	NIST Webbook
hfus	11.24	kJ/mol	Joback Method
hvap	50.20 ± 0.10	kJ/mol	NIST Webbook
hvap	50.22	kJ/mol	NIST Webbook
ie	8.66	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
ie	8.61	eV	NIST Webbook
ie	8.71	eV	NIST Webbook
ie	8.35	eV	NIST Webbook
ie	8.30 ± 0.10	eV	NIST Webbook
log10ws	-2.55		Crippen Method
logp	2.564		Crippen Method
mcvol	103.050	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
rinpol	1002.00		NIST Webbook

rinpol	1020.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	140.40		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	995.00		NIST Webbook
ripol	1375.00		NIST Webbook
ripol	1414.00		NIST Webbook
ripol	1377.00		NIST Webbook
tb	444.00 ± 4.00	K	NIST Webbook
tb	438.00 ± 3.00	K	NIST Webbook
tb	443.65 ± 2.00	K	NIST Webbook
tc	663.97	K	Joback Method
tf	235.55	K	Joback Method
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.52	J/mol×K	438.74	Joback Method
cpg	215.03	J/mol×K	476.28	Joback Method
cpg	229.41	J/mol×K	513.82	Joback Method
cpg	242.73	J/mol×K	551.36	Joback Method
cpg	255.05	J/mol×K	588.89	Joback Method
cpg	266.45	J/mol×K	626.43	Joback Method
cpg	277.00	J/mol×K	663.97	Joback Method
dvisc	0.0014956	Pa×s	235.55	Joback Method
dvisc	0.0010430	Pa×s	269.42	Joback Method
dvisc	0.0007883	Pa×s	303.28	Joback Method
dvisc	0.0006303	Pa×s	337.14	Joback Method
dvisc	0.0005250	Pa×s	371.01	Joback Method
dvisc	0.0004508	Pa×s	404.88	Joback Method
dvisc	0.0003963	Pa×s	438.74	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source

tbrp	446.80	K	100.00	NIST Webbook
tbrp	353.20	K	4.90	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=C873494&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
ripol:	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