Benzene, 2,2-dichlorocyclopropyl-

Other names: (2,2-Dichlorocyclopropyl)-benzene
1,1-Dichloro-2-phenylcyclopropane
Cyclopropane, 1,1-dichloro, 2-phenyl
Inchi: InChI=1S/C9H8Cl2/c10-9(11)6-8(9)7-4-2-1-3-5-7/h1-5,8H,6H2
InchiKey: WLWFQGXZIDYWQF-UHFFFAOYSA-N
Formula: C9H8Cl2
SMILES: ClC1(Cl)CC1c1ccccc1
Mol. weight [g/mol]: 187.07
CAS: 2415-80-7

Physical Properties

Property code	Value	Unit	Source
gf	161.00	kJ/mol	Joback Method
hf	43.66	kJ/mol	Joback Method
hfus	14.41	kJ/mol	Joback Method
hvap	45.13	kJ/mol	Joback Method
ie	8.70	eV	NIST Webbook
ie	8.97	eV	NIST Webbook
log10ws	-3.46		Crippen Method
logp	3.348		Crippen Method
mcvol	127.530	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
rinpol	1260.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1261.00		NIST Webbook
ripol	1789.00		NIST Webbook
ripol	1789.00		NIST Webbook
tb	509.17	K	Joback Method
tc	757.06	K	Joback Method
tf	315.05	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.18	J/mol×K	509.17	Joback Method
cpg	268.79	J/mol×K	550.49	Joback Method
cpg	281.04	J/mol×K	591.80	Joback Method
cpg	292.17	J/mol×K	633.12	Joback Method
cpg	302.37	J/mol×K	674.43	Joback Method
cpg	311.87	J/mol×K	715.75	Joback Method
cpg	320.88	J/mol×K	757.06	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.20	K	1.30	NIST Webbook

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=C2415807&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
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