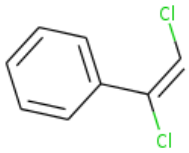
1,2-dichloro-1-phenylethylene

Other names: 1,2-Dichloro-1-phenylethene; 1,2-dichloro-1-phenylethylene; Benzene, (1,2-dichloroethenyl)-; Dichlorostyrene; Dwuchlorostyren; Styrene, «alpha»,«beta»-dichloro-.
InChI: InChI=1S/C8H6Cl2/c9-6-8(10)7-4-2-1-3-5-7/h1-6H/b8-6+
InChI Key: OQGSCHGFHOSXFY-SOFGYWHQSA-N
Formula: C8H6Cl2
SMILES: ClC=C(Cl)c1ccccc1
Molecular Weight: 173.04
CAS: 6607-45-0



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	176.70	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	104.03	kJ/mol	Joback Method
$\Delta_{fus} H°$	17.80	kJ/mol	Joback Method
$\Delta_{vap} H°$	44.49	kJ/mol	Joback Method
$log P_{oct/wat}$	3.46		Crippen Method
P_c	3577.07	kPa	Joback Method
T_{boil}	488.02	K	Joback Method
T_c	727.10	K	Joback Method
T_{fus}	247.14	K	Joback Method
V_c	0.45	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	209.12	J/mol×K	488.02	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H6Cl2/c9-6-8(10)7-4-2-1-3-5-7/h1-6H/b8-6+
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
***log*$P_{oct/wat}$**: Octanol/Water partition coefficient .
P_c: Critical Pressure (kPa).
T_{boil}: Normal Boiling Point Temperature (K).
T_c: Critical Temperature (K).
T_{fus}: Normal melting (fusion) point (K).
V_c: Critical Volume (m^3/kg-mol).