2-Chlorostyrene

Other names:	1-Chloro-2-vinylbenzene
	Benzene, 1-chloro-2-ethenyl-
	Styrene, o-chloro-
	o-Chlorostyrene
Inchi:	InChI=1S/C8H7Cl/c1-2-7-5-3-4-6-8(7)9/h2-6H,1H2
InchiKey:	ISRGONDNXBCDBM-UHFFFAOYSA-N
Formula:	C8H7Cl
SMILES:	C=Cc1ccccc1Cl
Mol. weight [g/mol]:	138.59
CAS:	2039-87-4

Physical Properties

Property code	Value	Unit	Source
gf	195.17	kJ/mol	Joback Method
hf	126.30	kJ/mol	Joback Method
hfus	13.04	kJ/mol	Joback Method
hvap	40.06	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.983		Crippen Method
mcvol	107.760	ml/mol	McGowan Method
pc	3607.21	kPa	Joback Method
tb	461.90	K	NIST Webbook
tc	671.47	K	Joback Method
tf	247.02	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.74	J/mol×K	671.47	Joback Method
cpg	186.15	J/mol×K	448.21	Joback Method
cpg	197.08	J/mol×K	485.42	Joback Method
cpg	207.30	J/mol×K	522.63	Joback Method
cpg	216.84	J/mol×K	559.84	Joback Method

cpg	225.74	J/mol×K	597.05	Joback Method
cpg	234.03	J/mol×K	634.26	Joback Method
dvisc	0.0002538	Pa×s	448.21	Joback Method
dvisc	0.0020587	Pa×s	247.02	Joback Method
dvisc	0.0011790	Pa×s	280.55	Joback Method
dvisc	0.0007605	Pa×s	314.08	Joback Method
dvisc	0.0005339	Pa×s	347.62	Joback Method
dvisc	0.0003989	Pa×s	381.15	Joback Method
dvisc	0.0003124	Pa×s	414.68	Joback Method
hvapt	46.00	kJ/mol	443.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	332.20	K	0.90	NIST Webbook
tbrp	337.80	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46526e+01
Coeff. B	-4.16255e+03
Coeff. C	-4.70680e+01
Temperature range (K), min.	336.84
Temperature range (K), max.	492.68

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=C2039874&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume