

Benzene, 1-chloro-3-ethenyl-

Other names:	3-Chlorostyrene 3-ClC ₆ H ₄ CH=CH ₂ Styrene, m-chloro- m-Chlorostyrene
Inchi:	InChI=1S/C ₈ H ₇ Cl/c1-2-7-4-3-5-8(9)6-7/h2-6H,1H ₂
InchiKey:	BOVQCIDBZXNFEJ-UHFFFAOYSA-N
Formula:	C ₈ H ₇ Cl
SMILES:	C=Cc1cccc(Cl)c1
Mol. weight [g/mol]:	138.59
CAS:	2039-85-2

Physical Properties

Property code	Value	Unit	Source
affp	841.50	kJ/mol	NIST Webbook
basg	812.60	kJ/mol	NIST Webbook
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	448.21	K	Joback Method
tc	671.47	K	Joback Method
tf	247.02	K	Joback Method
vc	0.406	m ³ /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	Paxs	448.21	Joback Method
dvisc	0.0020587	Paxs	247.02	Joback Method
dvisc	0.0011790	Paxs	280.55	Joback Method
dvisc	0.0007605	Paxs	314.08	Joback Method
dvisc	0.0005339	Paxs	347.62	Joback Method
dvisc	0.0003989	Paxs	381.15	Joback Method
dvisc	0.0003124	Paxs	414.68	Joback Method
hvapt	46.10	kJ/mol	380.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.51967e+01
Coeff. B	-4.45746e+03
Coeff. C	-4.16230e+01
Temperature range (K), min.	340.60
Temperature range (K), max.	492.55

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C2039852&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

affp: Proton affinity

basg:	Gas basicity
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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