Benzene, 1,4-dichloro-2-ethenyl-

Other names:	2,5-Dichlorostyrene
	Benzene, 1,4-dichoro-2-ethenyl-
	Styrene, 2,5-dichloro-
Inchi:	InChI=1S/C8H6Cl2/c1-2-6-5-7(9)3-4-8(6)10/h2-5H,1H2
InchiKey:	IZMZREOTRMMCCB-UHFFFAOYSA-N
Formula:	C8H6Cl2
SMILES:	C=Cc1cc(Cl)ccc1Cl
Mol. weight [g/mol]:	173.04
CAS:	1123-84-8

Physical Properties

Property code	Value	Unit	Source
chl	-4088.30	kJ/mol	NIST Webbook
gf	173.61	kJ/mol	Joback Method
hf	99.09	kJ/mol	Joback Method
hfl	35.00 ± 2.00	kJ/mol	NIST Webbook
hfus	16.85	kJ/mol	Joback Method
hvap	45.10	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.636		Crippen Method
mcvol	120.000	ml/mol	McGowan Method
pc	3392.03	kPa	Joback Method
tb	490.62	K	Joback Method
tc	721.44	K	Joback Method
tf	289.46	K	Joback Method
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.24	J/mol×K	490.62	Joback Method
cpg	219.01	J/mol×K	529.09	Joback Method
cpg	228.14	J/mol×K	567.56	Joback Method
cpg	236.64	J/mol×K	606.03	Joback Method

cpg	244.54	J/mol×K	644.50	Joback Method
cpg	251.90	J/mol×K	682.97	Joback Method
cpg	258.72	J/mol×K	721.44	Joback Method
dvisc	0.0016081	Pa×s	289.46	Joback Method
dvisc	0.0010190	Pa×s	322.99	Joback Method
dvisc	0.0007036	Pa×s	356.51	Joback Method
dvisc	0.0005178	Pa×s	390.04	Joback Method
dvisc	0.0004000	Pa×s	423.57	Joback Method
dvisc	0.0003209	Pa×s	457.09	Joback Method
dvisc	0.0002653	Pa×s	490.62	Joback Method
hvapt	54.30	kJ/mol	414.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	345.70	K	0.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53048e+01
Coeff. B	-4.93971e+03
Coeff. C	-4.13450e+01
Temperature range (K), min.	329.00
Temperature range (K), max.	535.65

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1123848&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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

Legend

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
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

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