

2,6-Dichlorostyrene

Other names:	1,3-Dichloro-2-vinylbenzene Benzene, 1,3-dichloro-2-ethenyl-
Inchi:	InChI=1S/C8H6Cl2/c1-2-6-7(9)4-3-5-8(6)10/h2-5H,1H2
InchiKey:	YJCVRMIJBXTMNR-UHFFFAOYSA-N
Formula:	C8H6Cl2
SMILES:	C=Cc1c(Cl)cccc1Cl
Mol. weight [g/mol]:	173.04
CAS:	28469-92-3

Physical Properties

Property code	Value	Unit	Source
gf	173.61	kJ/mol	Joback Method
hf	99.09	kJ/mol	Joback Method
hfus	16.85	kJ/mol	Joback Method
hvap	53.80 ± 1.50	kJ/mol	NIST Webbook
ie	8.70 ± 0.02	eV	NIST Webbook
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/molxK	490.62	Joback Method
cpg	219.01	J/molxK	529.09	Joback Method
cpg	228.14	J/molxK	567.56	Joback Method
cpg	236.64	J/molxK	606.03	Joback Method
cpg	244.54	J/molxK	644.50	Joback Method
cpg	251.90	J/molxK	682.97	Joback Method

cpg	258.72	J/molxK	721.44	Joback Method
dvisc	0.0016081	Paxs	289.46	Joback Method
dvisc	0.0010190	Paxs	322.99	Joback Method
dvisc	0.0007036	Paxs	356.51	Joback Method
dvisc	0.0005178	Paxs	390.04	Joback Method
dvisc	0.0004000	Paxs	423.57	Joback Method
dvisc	0.0003209	Paxs	457.09	Joback Method
dvisc	0.0002653	Paxs	490.62	Joback Method
hvapt	50.40	kJ/mol	405.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	362.20	K	1.00	NIST Webbook
tbrp	337.70	K	0.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.51217e+01
Coeff. B	-4.91656e+03
Coeff. C	-3.54940e+01
Temperature range (K), min.	362.15
Temperature range (K), max.	536.66

Sources

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=C28469923&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/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
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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