1,3-Dichloro-5-vinylbenzene

Other names: 3,5-Dichlorostyrene
Inchi: InChI=1S/C8H6Cl2/c1-2-6-3-7(9)5-8(10)4-6/h2-5H,1H2
InchiKey: RVZNTKZAFRNXIK-UHFFFAOYSA-N
Formula: C8H6Cl2
SMILES: C=Cc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]: 173.04
CAS: 2155-42-2

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	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	55.10	kJ/mol	412.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55279e+01
Coeff. B	-5.13464e+03
Coeff. C	-3.29340e+01
Temperature range (K), min.	369.84
Temperature range (K), max.	535.52

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2155422&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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