

1,2,2-Trichloro-1-phenylethene

Other names:	(trichlorovinyl)benzene 1,2,2-Trichloro-1-phenylethene styrene, «alpha»,«beta»,«beta»-trichloro-
Inchi:	InChI=1S/C8H5Cl3/c9-7(8(10)11)6-4-2-1-3-5-6/h1-5H
InchiKey:	SVHAMPNLOLKSFU-UHFFFAOYSA-N
Formula:	C8H5Cl3
SMILES:	ClC(Cl)=C(Cl)c1ccccc1
Mol. weight [g/mol]:	207.49

Physical Properties

Property code	Value	Unit	Source
af	0.3218		Cheméo Relay (1.0)
gf	156.22	kJ/mol	Joback Method
hf	98.78	kJ/mol	Cheméo Relay (1.0)
hfus	20.69	kJ/mol	Joback Method
hvap	55.62	kJ/mol	Cheméo Relay (1.0)
ie	8.60	eV	Cheméo Relay (1.0)
log10ws	-3.89		Cheméo Relay (1.0)
logp	4.029		Crippen Method
mcvol	132.240	ml/mol	McGowan Method
pc	3443.98	kPa	Joback Method
tb	510.94	K	Cheméo Relay (1.0)
tc	745.61	K	Cheméo Relay (1.0)
tf	280.08	K	Cheméo Relay (1.0)
vc	0.466	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.49	J/mol×K	525.33	Joback Method
cpg	241.71	J/mol×K	566.87	Joback Method
cpg	251.00	J/mol×K	608.42	Joback Method
cpg	259.42	J/mol×K	649.96	Joback Method
cpg	267.05	J/mol×K	691.51	Joback Method

cpg	273.99	J/mol×K	733.05	Joback Method
cpg	280.30	J/mol×K	774.60	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C700607&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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