

Benzene, (2-chloroethenyl)-

Other names:	Styrene, «beta»-chloro- «beta»-Chlorostyrene 1-Chloro-2-phenylethene «omega»-Chloro styrene 2-Chloro-1-phenylethene 2-Chloroethenyl]benzene (2-chlorovinyl)benzene
Inchi:	InChI=1S/C8H7Cl/c9-7-6-8-4-2-1-3-5-8/h1-7H/b7-6+
InchiKey:	SBYMUUGTIKLCR-VOTSOKGWSA-N
Formula:	C8H7Cl
SMILES:	ClC=Cc1ccccc1
Mol. weight [g/mol]:	138.59
CAS:	622-25-3

Physical Properties

Property code	Value	Unit	Source
gf	197.18	kJ/mol	Joback Method
hf	129.56	kJ/mol	Joback Method
hfus	14.92	kJ/mol	Joback Method
hvap	40.02	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.896		Crippen Method
mcvol	107.760	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
rinpol	1030.00		NIST Webbook
tb	450.71	K	Joback Method
tc	678.78	K	Joback Method
tf	231.18	K	Joback Method
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.30	J/mol×K	450.71	Joback Method

cpg	197.01	J/mol×K	488.72	Joback Method
cpg	207.83	J/mol×K	526.73	Joback Method
cpg	217.84	J/mol×K	564.74	Joback Method
cpg	227.07	J/mol×K	602.75	Joback Method
cpg	235.59	J/mol×K	640.77	Joback Method
cpg	243.46	J/mol×K	678.78	Joback Method
dvisc	0.0030816	Pa×s	231.18	Joback Method
dvisc	0.0014766	Pa×s	267.77	Joback Method
dvisc	0.0008445	Pa×s	304.36	Joback Method
dvisc	0.0005445	Pa×s	340.95	Joback Method
dvisc	0.0003822	Pa×s	377.53	Joback Method
dvisc	0.0002856	Pa×s	414.12	Joback Method
dvisc	0.0002238	Pa×s	450.71	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	361.50 ± 0.50	K	2.30	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C622253&Units=SI
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

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
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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