Benzene, (2-chloroethyl)-

Other names:	(2-Chloroethyl)benzene
	(«beta»-Chloroethyl)benzene
	(Â«betaÂ»-Chloroethyl)benzene
	1-Chloro-2-phenylethane
	2-Phenyl-1-chloroethane
	2-Phenylethyl chloride
	NSC 27886
	Phenethyl chloride
	«beta»-Phenethyl chloride
	«beta»-Phenylethyl chloride
	Â«betaÂ»-Phenethyl chloride
	Â«betaÂ»-Phenylethyl chloride
Inchi:	InChI=1S/C8H9Cl/c9-7-6-8-4-2-1-3-5-8/h1-5H,6-7H2
InchiKey:	MNNZINNZIQVULG-UHFFFAOYSA-N
Formula:	C8H9Cl
SMILES:	ClCCc1ccccc1
Mol. weight [g/mol]:	140.61
CAS:	622-24-2

Physical Properties

Property code	Value	Unit	Source
gf	116.96	kJ/mol	Joback Method
hf	12.34	kJ/mol	Joback Method
hfus	14.71	kJ/mol	Joback Method
hvap	40.06	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.468		Crippen Method
mcvol	112.060	ml/mol	McGowan Method
pc	3493.01	kPa	Joback Method
rinpol	1081.00		NIST Webbook
rinpol	1082.60		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	167.20		NIST Webbook
rinpol	1076.00		NIST Webbook
ripol	1593.00		NIST Webbook

tb	446.55	K	Joback Method
tc	663.28	K	Joback Method
tf	236.26	K	Joback Method
vc	0.424	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.53	J/mol×K	627.16	Joback Method
cpg	236.11	J/mol×K	554.92	Joback Method
cpg	225.38	J/mol×K	518.79	Joback Method
cpg	213.93	J/mol×K	482.67	Joback Method
cpg	201.71	J/mol×K	446.55	Joback Method
cpg	246.15	J/mol×K	591.04	Joback Method
cpg	264.28	J/mol×K	663.28	Joback Method
dvisc	0.0033558	Pa×s	236.26	Joback Method
dvisc	0.0002678	Pa×s	446.55	Joback Method
dvisc	0.0003411	Pa×s	411.50	Joback Method
dvisc	0.0004544	Pa×s	376.45	Joback Method
dvisc	0.0006422	Pa×s	341.41	Joback Method
dvisc	0.0009824	Pa×s	306.36	Joback Method
dvisc	0.0016772	Pa×s	271.31	Joback Method
hvapt	53.10	kJ/mol	418.00	NIST Webbook
hvapt	51.70	kJ/mol	368.00	NIST Webbook
rhol	1066.91	kg/m3	298.15	Excess Enthalpies of Chloroalkylbenzene + Alkylbenzene Mixtures

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	356.20	K	2.10	NIST Webbook
tbrp	365.20	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49195e+01
Coeff. B	-4.01689e+03
Coeff. C	-7.19910e+01
Temperature range (K), min.	346.52
Temperature range (K), max.	490.07

Sources

Excess Enthalpies of Chloroalkylbenzene + Alkylbenzene Mixtures:	https://www.doi.org/10.1021/je7002447
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=C622242&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

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
rhol:	Liquid Density

rinpol:	Non-polar retention indices
ripol:	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