Benzene, (1-chloroethyl)-

Other names:	(1-Chloroethyl)benzene
	(«alpha»-Chloroethyl)benzene
	(Â«alphaÂ»-Chloroethyl)benzene
	1-Chloro-1-phenylethane
	1-Phenyl-1-chloroethane
	1-Phenylethyl chloride
	«alpha»-Methylbenzyl chloride
	«alpha»-Phenethyl chloride
	«alpha»-Phenylethyl chloride
	Â«alphaÂ»-Methylbenzyl chloride
	Â«alphaÂ»-Phenethyl chloride
	Â«alphaÂ»-Phenylethyl chloride
Inchi:	InChI=1S/C8H9Cl/c1-7(9)8-5-3-2-4-6-8/h2-7H,1H3
InchiKey:	GTLWADFFABIGAE-UHFFFAOYSA-N
Formula:	C8H9Cl
SMILES:	CC(Cl)c1ccccc1
Mol. weight [g/mol]:	140.61
CAS:	672-65-1

Physical Properties

Property code	Value	Unit	Source
chl	-4399.77	kJ/mol	NIST Webbook
gf	114.52	kJ/mol	Joback Method
hf	7.06	kJ/mol	Joback Method
hfl	-58.24	kJ/mol	NIST Webbook
hfus	11.19	kJ/mol	Joback Method
hvap	52.80 ± 0.20	kJ/mol	NIST Webbook
hvap	52.40	kJ/mol	NIST Webbook
log10ws	-2.89		Crippen Method
logp	2.986		Crippen Method
mcvol	112.060	ml/mol	McGowan Method
pc	3526.27	kPa	Joback Method
rinpol	1051.00		NIST Webbook
rinpol	1039.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1060.00		NIST Webbook

rinpol	1051.00		NIST Webbook
tb	446.11	K	Joback Method
tc	668.17	K	Joback Method
tf	221.26	K	Joback Method
vc	0.418	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.83	J/mol×K	446.11	Joback Method
cpg	214.45	J/mol×K	483.12	Joback Method
cpg	226.25	J/mol×K	520.13	Joback Method
cpg	237.29	J/mol×K	557.14	Joback Method
cpg	247.59	J/mol×K	594.15	Joback Method
cpg	257.18	J/mol×K	631.16	Joback Method
cpg	266.11	J/mol×K	668.17	Joback Method
dvisc	0.0021308	Pa×s	258.74	Joback Method
dvisc	0.0050108	Pa×s	221.26	Joback Method
dvisc	0.0011250	Pa×s	296.21	Joback Method
dvisc	0.0006856	Pa×s	333.69	Joback Method
dvisc	0.0004617	Pa×s	371.16	Joback Method
dvisc	0.0003344	Pa×s	408.63	Joback Method
dvisc	0.0002556	Pa×s	446.11	Joback Method
hvapt	51.40	kJ/mol	354.00	NIST Webbook
hvapt	47.00	kJ/mol	360.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	361.50 ± 0.50	K	4.50	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42544e+01
Coeff. B	-3.77816e+03
Coeff. C	-6.98500e+01
Temperature range (K), min.	340.36
Temperature range (K), max.	492.32

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C672651&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

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
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