1,3-Butadiene, 2-chloro-

Other names:	2-CHLORO-1,3-BUTADIENE
	2-CHLOROBUTADIENE
	2-Chloor-1,3-butadieen
	2-Chlor-1,3-butadien
	2-Chlorobuta-1,3-diene
	2-Chlorobutadiene 1,3
	2-Chloroprene
	2-Cloro-1,3-butadiene
	Chlorobutadiene
	Chloropreen
	Chloropren
	Chloroprene
	Cloroprene
	NSC 18589
	Neoprene
	UN 1991
	«beta»-Chlorobutadiene
	«beta»-Chloroprene
	Â«betaÂ»-Chlorobutadiene
	Â«betaÂ»-Chloroprene
Inchi:	InChI=1S/C4H5Cl/c1-3-4(2)5/h3H,1-2H2
InchiKey:	YACLQRRMGMJLJV-UHFFFAOYSA-N
Formula:	C4H5Cl
SMILES:	C=CC(=C)Cl
Mol. weight [g/mol]:	88.54
CAS:	126-99-8

Physical Properties

Property code	Value	Unit	Source
gf	138.00	kJ/mol	Joback Method
hf	99.44	kJ/mol	Joback Method
hfus	6.44	kJ/mol	Joback Method
hvap	27.62	kJ/mol	Joback Method
ie	8.83 ± 0.01	eV	NIST Webbook
log10ws	-1.85		Crippen Method
logp	1.925		Crippen Method
mcvol	70.860	ml/mol	McGowan Method

nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
pc	4162.33	kPa	Joback Method
rinpol	572.00		NIST Webbook
rinpol	550.00		NIST Webbook
rinpol	557.00		NIST Webbook
rinpol	572.00		NIST Webbook
rinpol	550.00		NIST Webbook
tb	332.60	K	NIST Webbook
tc	505.37	K	Joback Method
tf	147.28	K	Joback Method
vc	0.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	94.79	J/mol×K	321.59	Joback Method
cpg	100.97	J/mol×K	352.22	Joback Method
cpg	106.81	J/mol×K	382.85	Joback Method
cpg	112.35	J/mol×K	413.48	Joback Method
cpg	117.58	J/mol×K	444.11	Joback Method
cpg	122.52	J/mol×K	474.74	Joback Method
cpg	127.19	J/mol×K	505.37	Joback Method
hvapt	29.60	kJ/mol	253.00	NIST Webbook
hvapt	29.60	kJ/mol	306.00	NIST Webbook
hvapt	30.90	kJ/mol	313.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46039e+01
Coeff. B	-3.21417e+03
Coeff. C	-1.07170e+01
Temperature range (K), min.	235.23
Temperature range (K), max.	356.61

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.65883e+01
Coeff. B	-4.90047e+03
Coeff. C	-4.74673e+00
Coeff. D	2.93952e-06
Temperature range (K), min.	143.15
Temperature range (K), max.	525.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C126998&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1746
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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1746.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure

pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume