

2-Chloro-1-butene

Other names:	1-Butene, 2-chloro- 2-chlorobut-1-ene
Inchi:	InChI=1S/C4H7Cl/c1-3-4(2)5/h2-3H2,1H3
InchiKey:	HSEFPJMMKNHABB-UHFFFAOYSA-N
Formula:	C4H7Cl
SMILES:	C=C(Cl)CC
Mol. weight [g/mol]:	90.55
CAS:	2211-70-3

Physical Properties

Property code	Value	Unit	Source
gf	50.16	kJ/mol	Joback Method
hf	-29.30	kJ/mol	NIST Webbook
hfus	7.72	kJ/mol	Joback Method
hvap	28.29	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	2.149		Crippen Method
mcvol	75.160	ml/mol	McGowan Method
pc	3945.61	kPa	Joback Method
tb	331.70	K	NIST Webbook
tb	331.65 ± 1.00	K	NIST Webbook
tb	331.65 ± 1.00	K	NIST Webbook
tc	504.71	K	Joback Method
tf	149.04	K	Joback Method
vc	0.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	106.79	J/mol×K	324.91	Joback Method
cpg	113.69	J/mol×K	354.88	Joback Method
cpg	120.28	J/mol×K	384.84	Joback Method
cpg	126.57	J/mol×K	414.81	Joback Method
cpg	132.58	J/mol×K	444.78	Joback Method

cpg	138.32	J/mol×K	474.75	Joback Method
cpg	143.79	J/mol×K	504.71	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.32936e+01
Coeff. B	-2.18238e+03
Coeff. C	-8.01360e+01
Temperature range (K), min.	247.93
Temperature range (K), max.	353.55

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2211703&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

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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