

1,3-Butadiene, 2-chloro-3-methyl-

Other names:	2-chloro-3-methyl-1,3-butadiene
Inchi:	InChI=1S/C5H7Cl/c1-4(2)5(3)6/h1,3H2,2H3
InchiKey:	PKVRTDNAPQGMGP-UHFFFAOYSA-N
Formula:	C5H7Cl
SMILES:	C=C(C)C(=C)Cl
Mol. weight [g/mol]:	102.56
CAS:	1809-02-5

Physical Properties

Property code	Value	Unit	Source
gf	137.87	kJ/mol	Joback Method
hf	69.01	kJ/mol	Joback Method
hfus	7.72	kJ/mol	Joback Method
hvap	29.93	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	2.315		Crippen Method
mcvol	84.950	ml/mol	McGowan Method
pc	3713.49	kPa	Joback Method
rinpol	683.00		NIST Webbook
tb	344.35	K	Joback Method
tc	532.11	K	Joback Method
tf	144.59	K	Joback Method
vc	0.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	125.33	J/mol×K	344.35	Joback Method
cpg	133.25	J/mol×K	375.64	Joback Method
cpg	140.75	J/mol×K	406.94	Joback Method
cpg	147.86	J/mol×K	438.23	Joback Method
cpg	154.59	J/mol×K	469.52	Joback Method
cpg	160.95	J/mol×K	500.81	Joback Method
cpg	166.98	J/mol×K	532.11	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.35725e+01
Coeff. B	-2.94898e+03
Coeff. C	-4.29400e+01
Temperature range (K), min.	264.92
Temperature range (K), max.	399.92

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1809025&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
mcvol:	McGowan's characteristic volume
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

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