1-Butene, 3,4-dichloro-

Other names:	1,2-DICHLORO-3-BUTENE
	1,2-Dichlorobut-3-ene
	3,4-DICHLORO-1-BUTENE
	3,4-dichlorobut-1-ene
Inchi:	InChI=1S/C4H6Cl2/c1-2-4(6)3-5/h2,4H,1,3H2
InchiKey:	XVEASTGLHPVZNA-UHFFFAOYSA-N
Formula:	C4H6Cl2
SMILES:	C=CC(Cl)CCl
Mol. weight [g/mol]:	125.00
CAS:	760-23-6

Physical Properties

Property code	Value	Unit	Source
gf	44.34	kJ/mol	Joback Method
hf	-37.22	kJ/mol	Joback Method
hfus	9.71	kJ/mol	Joback Method
hvap	32.21	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	2.019		Crippen Method
mcvol	87.400	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
rinpol	769.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	769.00		NIST Webbook
tb	427.00 ± 3.00	K	NIST Webbook
tb	396.20	K	NIST Webbook
tc	552.53	K	Joback Method
tf	212.00 ± 5.00	K	NIST Webbook
vc	0.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	164.58	J/mol×K	552.53	Joback Method

cpg	159.34	J/mol×K	520.78	Joback Method
cpg	153.80	J/mol×K	489.03	Joback Method
cpg	147.94	J/mol×K	457.28	Joback Method
cpg	141.75	J/mol×K	425.52	Joback Method
cpg	135.22	J/mol×K	393.77	Joback Method
cpg	128.34	J/mol×K	362.02	Joback Method
dvisc	0.0057370	Pa×s	177.92	Joback Method
dvisc	0.0003269	Pa×s	362.02	Joback Method
dvisc	0.0004224	Pa×s	331.34	Joback Method
dvisc	0.0005753	Pa×s	300.65	Joback Method
dvisc	0.0008403	Pa×s	269.97	Joback Method
dvisc	0.0013527	Pa×s	239.29	Joback Method
dvisc	0.0025049	Pa×s	208.60	Joback Method
hvapt	38.00	kJ/mol	358.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43660e+01
Coeff. B	-3.38424e+03
Coeff. C	-4.90140e+01
Temperature range (K), min.	289.40
Temperature range (K), max.	422.78

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.43058e+01
Coeff. B	-6.68656e+03
Coeff. C	-7.22337e+00
Coeff. D	3.92607e-06
Temperature range (K), min.	212.00
Temperature range (K), max.	589.00

Sources

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/research/kdb/hcprop/showprop.php?cmpid=1752
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C760236&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=1752

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