

(E)-1-chlorobut-2-ene

Other names:	2-Butene, 1-chloro-, (E)-
Inchi:	InChI=1S/C4H7Cl/c1-2-3-4-5/h2-3H,4H2,1H3/b3-2+
InchiKey:	YTKRILODNOEEX-NSCUHMNNSA-N
Formula:	C4H7Cl
SMILES:	CC=CCCl
Mol. weight [g/mol]:	90.55
CAS:	4894-61-5

Physical Properties

Property code	Value	Unit	Source
gf	51.09	kJ/mol	Joback Method
hf	-43.10	kJ/mol	NIST Webbook
hfus	10.51	kJ/mol	Joback Method
hvap	28.84	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.801		Crippen Method
mcvol	75.160	ml/mol	McGowan Method
pc	3970.51	kPa	Joback Method
tb	346.70	K	NIST Webbook
tc	514.66	K	Joback Method
tf	159.68	K	Joback Method
vc	0.288	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	104.96	J/mol×K	332.51	Joback Method
cpg	137.47	J/mol×K	484.30	Joback Method
cpg	131.63	J/mol×K	453.95	Joback Method
cpg	125.48	J/mol×K	423.59	Joback Method
cpg	118.99	J/mol×K	393.23	Joback Method
cpg	112.16	J/mol×K	362.87	Joback Method
cpg	143.01	J/mol×K	514.66	Joback Method
dvisc	0.0002244	Paxs	332.51	Joback Method

dvisc	0.0002848	Paxs	303.70	Joback Method
dvisc	0.0003798	Paxs	274.90	Joback Method
dvisc	0.0005418	Paxs	246.09	Joback Method
dvisc	0.0008494	Paxs	217.29	Joback Method
dvisc	0.0015278	Paxs	188.49	Joback Method
dvisc	0.0033962	Paxs	159.68	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	358.00	K	100.00	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4894615&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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