

(2E)-1-bromo-4-chloro-2-butene

Inchi:	InChI=1S/C4H6BrCl/c5-3-1-2-4-6/h1-2H,3-4H2/b2-1+
InchiKey:	KGRDKGJNOYVKPM-OWOJBTEDSA-N
Formula:	C4H6BrCl
SMILES:	C1CC=CCBr
Mol. weight [g/mol]:	169.45

Physical Properties

Property code	Value	Unit	Source
gf	65.41	kJ/mol	Joback Method
hf	1.92	kJ/mol	Joback Method
hfus	15.80	kJ/mol	Joback Method
hvap	35.28	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	2.176		Crippen Method
mcvol	92.660	ml/mol	McGowan Method
pc	4339.67	kPa	Joback Method
tb	398.67	K	Joback Method
tc	603.40	K	Joback Method
tf	219.48	K	Joback Method
vc	0.350	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	134.40	J/molxK	398.67	Joback Method
cpg	165.34	J/molxK	569.28	Joback Method
cpg	159.99	J/molxK	535.16	Joback Method
cpg	154.25	J/molxK	501.04	Joback Method
cpg	148.09	J/molxK	466.91	Joback Method
cpg	141.48	J/molxK	432.79	Joback Method
cpg	170.34	J/molxK	603.40	Joback Method
dvisc	0.0003370	Paxs	398.67	Joback Method
dvisc	0.0004230	Paxs	368.81	Joback Method
dvisc	0.0005527	Paxs	338.94	Joback Method

dvisc	0.0007604	Paxs	309.08	Joback Method
dvisc	0.0011202	Paxs	279.21	Joback Method
dvisc	0.0018108	Paxs	249.35	Joback Method
dvisc	0.0033355	Paxs	219.48	Joback Method

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=B6001195&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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