cis-2-Chloro-2-butene

Other names: 2-Butene, 2-chloro-, (Z)-
Inchi: InChI=1S/C4H7Cl/c1-3-4(2)5/h3H,1-2H3/b4-3-
InchiKey: DSDHFHLZEFQSFM-ARJAWSKDSA-N
Formula: C4H7Cl
SMILES: CC=C(C)Cl
Mol. weight [g/mol]: 90.55

Physical Properties

Property code	Value	Unit	Source
gf	42.54	kJ/mol	Joback Method
hf	-34.20	kJ/mol	Joback Method
hfus	9.21	kJ/mol	Joback Method
hvap	28.92	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	2.149		Crippen Method
mcvol	75.160	ml/mol	McGowan Method
pc	3995.65	kPa	Joback Method
rinpol	595.00		NIST Webbook
rinpol	595.00		NIST Webbook
tb	339.95 ± 1.00	K	NIST Webbook
tb	331.90	K	NIST Webbook
tb	339.95 ± 1.00	K	NIST Webbook
tc	518.49	K	Joback Method
tf	145.72	K	Joback Method
vc	0.289	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	105.03	J/mol×K	332.39	Joback Method
cpg	112.34	J/mol×K	363.41	Joback Method
cpg	119.28	J/mol×K	394.42	Joback Method
cpg	125.86	J/mol×K	425.44	Joback Method
cpg	132.09	J/mol×K	456.45	Joback Method

cpg	137.99	J/mol×K	487.47	Joback Method
cpg	143.59	J/mol×K	518.49	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C2211690&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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