

Trans-2-chloro-2-butene

Other names:	2-Butene, 2-chloro-, (E)- (E)-2-Butene, 2-fluoro
Inchi:	InChI=1S/C4H7Cl/c1-3-4(2)5/h3H,1-2H3/b4-3+
InchiKey:	DSDHFHLZEFQSFM-ONEGZZNKSA-N
Formula:	C4H7Cl
SMILES:	CC=C(C)Cl
Mol. weight [g/mol]:	90.55
CAS:	2211-68-9

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
mvol	75.160	ml/mol	McGowan Method
pc	3995.65	kPa	Joback Method
tb	334.65 ± 2.50	K	NIST Webbook
tb	338.15 ± 1.50	K	NIST Webbook
tb	335.75 ± 1.00	K	NIST Webbook
tb	335.75 ± 1.00	K	NIST Webbook
tc	518.49	K	Joback Method
tf	145.72	K	Joback Method
vc	0.289	m ³ /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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2211689&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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