(E)-1,3-Dichloro-2-butene

Other names: 2-Butene, 1,3-dichloro-, (2E)-
trans 1,3-dichloro-2-butene
Inchi: InChI=1S/C4H6Cl2/c1-4(6)2-3-5/h2H,3H2,1H3/b4-2+
InchiKey: WLIADPFXSACYLS-DUXPYHPUSA-N
Formula: C4H6Cl2
SMILES: CC(Cl)=CCCl
Mol. weight [g/mol]: 125.00
CAS: 7415-31-8

Physical Properties

Property code	Value	Unit	Source
gf	30.61	kJ/mol	Joback Method
hf	-49.94	kJ/mol	Joback Method
hfus	13.40	kJ/mol	Joback Method
hvap	33.31	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	2.368		Crippen Method
mcvol	87.400	ml/mol	McGowan Method
pc	3815.10	kPa	Joback Method
tb	369.82	K	Joback Method
tc	565.76	K	Joback Method
tf	175.64	K	Joback Method
vc	0.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	126.87	J/mol×K	369.82	Joback Method
cpg	133.93	J/mol×K	402.48	Joback Method
cpg	140.56	J/mol×K	435.13	Joback Method
cpg	146.81	J/mol×K	467.79	Joback Method
cpg	152.67	J/mol×K	500.45	Joback Method
cpg	158.19	J/mol×K	533.10	Joback Method
cpg	163.37	J/mol×K	565.76	Joback Method

hvapt	39.30	kJ/mol	353.50	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=C7415318&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume