2,3-Dichloro-1,3-butadiene

Inchi: InChI=1S/C4H4Cl2/c1-3(5)4(2)6/h1-2H2
InchiKey: LIFLRQVHKGGNSG-UHFFFAOYSA-N
Formula: C4H4Cl2
SMILES: C=C(Cl)C(=C)Cl
Mol. weight [g/mol]: 122.98

Physical Properties

Property code	Value	Unit	Source
gf	117.52	kJ/mol	Joback Method
hf	73.91	kJ/mol	Joback Method
hfus	9.33	kJ/mol	Joback Method
hvap	32.09	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.491		Crippen Method
mcvol	83.100	ml/mol	McGowan Method
pc	3995.65	kPa	Joback Method
tb	358.90	K	Joback Method
tc	557.15	K	Joback Method
tf	163.24	K	Joback Method
vc	0.322	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	115.45	J/mol×K	358.90	Joback Method
cpg	121.48	J/mol×K	391.94	Joback Method
cpg	127.12	J/mol×K	424.98	Joback Method
cpg	132.40	J/mol×K	458.03	Joback Method
cpg	137.34	J/mol×K	491.07	Joback Method
cpg	141.96	J/mol×K	524.11	Joback Method
cpg	146.27	J/mol×K	557.15	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1745.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume