Benzene, 1-(1-methylethenyl)-2,4-dichloro-

Inchi: InChI=1S/C9H8Cl2/c1-6(2)8-4-3-7(10)5-9(8)11/h3-5H,1H2,2H3
InchiKey: AHDKLICOZGCVTI-UHFFFAOYSA-N
Formula: C9H8Cl2
SMILES: C=C(C)c1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 187.07
CAS: 104517-04-6

Physical Properties

Property code	Value	Unit	Source
gf	173.48	kJ/mol	Joback Method
hf	68.66	kJ/mol	Joback Method
hfus	18.13	kJ/mol	Joback Method
hvap	47.41	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	4.026		Crippen Method
mcvol	134.090	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
tb	513.38	K	Joback Method
tc	744.65	K	Joback Method
tf	286.77	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.14	J/mol×K	513.38	Joback Method
cpg	261.32	J/mol×K	551.92	Joback Method
cpg	271.77	J/mol×K	590.47	Joback Method
cpg	281.51	J/mol×K	629.01	Joback Method
cpg	290.59	J/mol×K	667.56	Joback Method
cpg	299.04	J/mol×K	706.10	Joback Method
cpg	306.90	J/mol×K	744.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104517046&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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