1,1,2,4,4-pentachlorobuta-1,3-diene

Inchi: InChI=1S/C4HCl5/c5-2(4(8)9)1-3(6)7/h1H
InchiKey: WVFBDVFCOCLEFM-UHFFFAOYSA-N
Formula: C4HCl5
SMILES: ClC(Cl)=CC(Cl)=C(Cl)Cl
Mol. weight [g/mol]: 226.32

Physical Properties

Property code	Value	Unit	Source
gf	57.94	kJ/mol	Joback Method
hf	0.48	kJ/mol	Joback Method
hfus	23.58	kJ/mol	Joback Method
hvap	46.58	kJ/mol	Joback Method
log10ws	-4.23		Aqueous Solubility Prediction Method
logp	4.191		Crippen Method
mcvol	119.820	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
tb	486.03	K	Joback Method
tc	724.46	K	Joback Method
tf	232.40	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.38	J/mol×K	486.03	Joback Method
cpg	173.20	J/mol×K	525.77	Joback Method
cpg	177.43	J/mol×K	565.51	Joback Method
cpg	181.15	J/mol×K	605.25	Joback Method
cpg	184.43	J/mol×K	644.99	Joback Method
cpg	187.33	J/mol×K	684.72	Joback Method
cpg	189.93	J/mol×K	724.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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