1,1,2,3-tetrachlorobuta-1,3-diene

Inchi: InChI=1S/C4H2Cl4/c1-2(5)3(6)4(7)8/h1H2
InchiKey: RCBKHVTUYAGMLB-UHFFFAOYSA-N
Formula: C4H2Cl4
SMILES: C=C(Cl)C(Cl)=C(Cl)Cl
Mol. weight [g/mol]: 191.87
CAS: 921-09-5

Physical Properties

Property code	Value	Unit	Source
gf	77.49	kJ/mol	Joback Method
hf	24.43	kJ/mol	Joback Method
hfus	17.90	kJ/mol	Joback Method
hvap	41.57	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.624		Crippen Method
mcvol	107.580	ml/mol	McGowan Method
pc	3713.49	kPa	Joback Method
tb	441.12	K	Joback Method
tc	666.86	K	Joback Method
tf	205.80	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.28	J/mol×K	441.12	Joback Method
cpg	157.68	J/mol×K	478.74	Joback Method
cpg	162.55	J/mol×K	516.37	Joback Method
cpg	166.95	J/mol×K	553.99	Joback Method
cpg	170.92	J/mol×K	591.61	Joback Method
cpg	174.50	J/mol×K	629.23	Joback Method
cpg	177.75	J/mol×K	666.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C921095&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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