2-Hexene, 4,5-dichloro-2,5-dimethyl-

Inchi: InChI=1S/C8H14Cl2/c1-6(2)5-7(9)8(3,4)10/h5,7H,1-4H3
InchiKey: OQGJAXHJJNMURO-UHFFFAOYSA-N
Formula: C8H14Cl2
SMILES: CC(C)=CC(Cl)C(C)(C)Cl
Mol. weight [g/mol]: 181.10
CAS: 22929-07-3

Physical Properties

Property code	Value	Unit	Source
gf	64.69	kJ/mol	Joback Method
hf	-146.53	kJ/mol	Joback Method
hfus	12.82	kJ/mol	Joback Method
hvap	40.53	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.577		Crippen Method
mcvol	143.760	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
tb	457.67	K	Joback Method
tc	664.18	K	Joback Method
tf	208.14	K	Joback Method
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.51	J/mol×K	457.67	Joback Method
cpg	292.36	J/mol×K	492.09	Joback Method
cpg	305.29	J/mol×K	526.51	Joback Method
cpg	317.37	J/mol×K	560.93	Joback Method
cpg	328.65	J/mol×K	595.35	Joback Method
cpg	339.17	J/mol×K	629.76	Joback Method
cpg	349.01	J/mol×K	664.18	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22929073&Units=SI
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