1,3-Pentadiene, 3-chloro-

Inchi: InChI=1S/C5H7Cl/c1-3-5(6)4-2/h3-4H,1H2,2H3/b5-4-
InchiKey: TVCSNURGFFKSMT-PLNGDYQASA-N
Formula: C5H7Cl
SMILES: C=CC(Cl)=CC
Mol. weight [g/mol]: 102.56
CAS: 37710-49-9

Physical Properties

Property code	Value	Unit	Source
gf	138.80	kJ/mol	Joback Method
hf	70.59	kJ/mol	Joback Method
hfus	10.51	kJ/mol	Joback Method
hvap	30.48	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	2.315		Crippen Method
mcvol	84.950	ml/mol	McGowan Method
pc	3736.23	kPa	Joback Method
rinpol	719.00		NIST Webbook
rinpol	719.00		NIST Webbook
tb	351.95	K	Joback Method
tc	541.93	K	Joback Method
tf	155.23	K	Joback Method
vc	0.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	123.88	J/mol×K	351.95	Joback Method
cpg	132.05	J/mol×K	383.61	Joback Method
cpg	139.75	J/mol×K	415.28	Joback Method
cpg	147.00	J/mol×K	446.94	Joback Method
cpg	153.83	J/mol×K	478.60	Joback Method
cpg	160.26	J/mol×K	510.26	Joback Method
cpg	166.31	J/mol×K	541.93	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37710499&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume