cis-Nonachlor

Other names:	4,7-Methano-1H-indene, 1,2,3,4,5,6,7,8,8-nonachloro-2,3,3a,4,7,7a-hexahydro-, (1«alpha»,2«alpha»,3«alpha»,3a«alpha»,4«beta»,7«beta»,7a«alpha»)- 4,7-Methanoindan, 1«alpha»,2«alpha»,3«alpha»,4«beta»,5,6,7«beta»,8,8-nonachloro-3a«alpha»,4,7,7a«alp Nonachlor, cis- c-Nonachlor
Inchi:	InChI=1S/C10H5Cl9/c11-3-1-2(4(12)5(3)13)9(17)7(15)6(14)8(1,16)10(9,18)19/h1-5H/t1-,
InchiKey:	OCHOKXCPKDPNQU-BBXWSCHTSA-N
Formula:	C10H5Cl9
SMILES:	ClC1=C(Cl)C2(Cl)C3C(Cl)C(Cl)C(Cl)C3C1(Cl)C2(Cl)Cl
Mol. weight [g/mol]:	444.22
CAS:	5103-73-1

Physical Properties

Property code	Value	Unit	Source
gf	51.78	kJ/mol	Joback Method
hf	-200.29	kJ/mol	Joback Method
hfus	38.64	kJ/mol	Joback Method
hvap	73.85	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	5.900		Crippen Method
mcvol	225.040	ml/mol	McGowan Method
pc	2224.99	kPa	Joback Method
rinpol	2216.10		NIST Webbook
rinpol	2216.10		NIST Webbook
rinpol	2257.90		NIST Webbook
ripol	3182.00		NIST Webbook
tb	776.05	K	Joback Method
tc	1055.67	K	Joback Method
tf	489.00 ± 0.20	K	NIST Webbook
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.89	J/mol×K	776.05	Joback Method

cpg	498.68	J/mol×K	822.65	Joback Method
cpg	513.14	J/mol×K	869.26	Joback Method
cpg	529.95	J/mol×K	915.86	Joback Method
cpg	549.84	J/mol×K	962.46	Joback Method
cpg	573.50	J/mol×K	1009.07	Joback Method
cpg	601.65	J/mol×K	1055.67	Joback Method
hvapt	83.80	kJ/mol	398.00	NIST Webbook

Sources

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=C5103731&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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