2,2,5-Endo,6-exo,8,9,9,10-octachlorobornane

Other names:	2,2,5,6-Tetrachloro-1,7-bis(chloromethyl)-7-(dichloromethyl)bicyclo[2.2.1]heptane, (5-endo,6-exo,7-syn)- 2,2,5-endo,6-exo,8,8,9,10-octachlorobornane 2,2,5-endo,6-exo,8c,9b,9c,10a-octachlorobornane Bicyclo[2.2.1]heptane, 2,2,5,6-tetrachloro-1,7-bis(chloromethyl)-7-(dichloromethyl)-, (5-endo,6-exo,7-syn)- Partial,420 rel-(1R,4R,5R,6R,7R)-2,2,5,6-tetrachloro-1,7-bis(chloromethyl)-7-(dichloromethyl)bicyclo[
Inchi:	InChI=1S/C10H10Cl8/c11-2-8(7(15)16)4-1-10(17,18)9(8,3-12)6(14)5(4)13/h4-7H,1-3H2
InchiKey:	YNEKMCSWRMRXIR-UHFFFAOYSA-N
Formula:	C10H10Cl8
SMILES:	ClCC1(C(Cl)Cl)C2CC(Cl)(Cl)C1(CCl)C(Cl)C2Cl
Mol. weight [g/mol]:	413.81
CAS:	58002-19-0

Physical Properties

Property code	Value	Unit	Source
gf	-2.47	kJ/mol	Joback Method
hf	-277.13	kJ/mol	Joback Method
hfus	31.27	kJ/mol	Joback Method
hvap	67.86	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	5.663		Crippen Method
mcvol	227.960	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpol	2373.20		NIST Webbook
rinpol	2373.20		NIST Webbook
tb	726.99	K	Joback Method
tc	988.40	K	Joback Method
tf	513.92	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.07	J/mol×K	726.99	Joback Method

cpg	520.99	J/mol×K	770.56	Joback Method
cpg	534.50	J/mol×K	814.13	Joback Method
cpg	549.15	J/mol×K	857.69	Joback Method
cpg	565.50	J/mol×K	901.26	Joback Method
cpg	584.12	J/mol×K	944.83	Joback Method
cpg	605.56	J/mol×K	988.40	Joback Method
pvap	1.51e-06	kPa	298.15	Vapor Pressures and Enthalpies of Vaporization for Toxaphene Congeners

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor Pressures and Enthalpies of Vaporization for Toxaphene Congeners	https://www.doi.org/10.1021/je020204q
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=C58002190&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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume