Bornane, 2,2,5-endo,6-exo,8,9,10-heptachloro-

Other names:	2,2,5,6-Tetrachloro-1,7,7-tris(chloromethyl)bicyclo[2.2.1]heptane, (5-endo,6-exo)- 2,2,5-endo,6-exo,8,9,10-heptachlorobornane 2,2,5-endo,6-exo,8c,9b,10a-heptachlorobornane 5-endo,6-exo-2,2,5,6-Tetrachloro-1,7,7-tris(chloromethyl)-bicyclo(2.2.1)heptane Bicyclo(2.2.1)heptane, 2,2,5,6-tetrachloro-1,7,7-tris(chloromethyl)-, (5-endo,6-exo)- Parlar 32 Sonatox Toxaphene 32 Toxaphene toxicant B rel-(1R,4R,5R,6R)-2,2,5,6-tetrachloro-1,7,7-tris(chloromethyl)bicyclo[2.2.1]heptane
Inchi:	InChI=1S/C10H11Cl7/c11-2-8(3-12)5-1-10(16,17)9(8,4-13)7(15)6(5)14/h5-7H,1-4H2
InchiKey:	IPVMCZLCKVSKGC-UHFFFAOYSA-N
Formula:	C10H11Cl7
SMILES:	ClCC1(CCl)C2CC(Cl)(Cl)C1(CCl)C(Cl)C2Cl
Mol. weight [g/mol]:	379.37
CAS:	51775-36-1

Physical Properties

Property code	Value	Unit	Source
gf	11.90	kJ/mol	Joback Method
hf	-256.11	kJ/mol	Joback Method
hfus	30.60	kJ/mol	Joback Method
hvap	63.86	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	5.098		Crippen Method
mcvol	215.720	ml/mol	McGowan Method
pc	2165.35	kPa	Joback Method
rinpol	2297.20		NIST Webbook
rinpol	2297.20		NIST Webbook
tb	690.00	K	Joback Method
tc	944.04	K	Joback Method
tf	499.00	K	Joback Method
vc	0.835	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.60	J/mol×K	690.00	Joback Method
cpg	498.45	J/mol×K	732.34	Joback Method
cpg	511.40	J/mol×K	774.68	Joback Method
cpg	524.96	J/mol×K	817.02	Joback Method
cpg	539.65	J/mol×K	859.36	Joback Method
cpg	555.98	J/mol×K	901.70	Joback Method
cpg	574.45	J/mol×K	944.04	Joback Method
pvap	2.82e-06	kPa	298.15	Vapor Pressures and Enthalpies of Vaporization for Toxaphene Congeners

Sources

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=C51775361&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
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