2-endo,3-exo,5-endo,6-exo,8,8,9,10-octachlorobor

Other names: rel-(2R,3R,5R,6R,7R)-2,3,5,6-tetrachloro-1,7-bis(chloromethyl)-7-(dichloromethyl)bicyclo[
Inchi: InChI=1S/C10H10Cl8/c11-1-9(2-12)3-4(13)6(15)10(9,8(17)18)7(16)5(3)14/h3-8H,1-2H2/t
InchiKey: JSAXRODSTJFHRO-GSSUXGFISA-N
Formula: C10H10Cl8
SMILES: ClCC1(CCl)C2C(Cl)C(Cl)C1(C(Cl)Cl)C(Cl)C2Cl
Mol. weight [g/mol]: 413.81

Physical Properties

Property code	Value	Unit	Source
gf	-4.69	kJ/mol	Joback Method
hf	-312.71	kJ/mol	Joback Method
hfus	38.64	kJ/mol	Joback Method
hvap	68.70	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	5.314		Crippen Method
mcvol	227.960	ml/mol	McGowan Method
pc	1964.82	kPa	Joback Method
rinpol	2258.40		NIST Webbook
tb	722.08	K	Joback Method
tc	974.16	K	Joback Method
tf	485.78	K	Joback Method
vc	0.878	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	584.28	J/mol×K	932.14	Joback Method
cpg	516.41	J/mol×K	722.08	Joback Method
cpg	529.47	J/mol×K	764.09	Joback Method
cpg	542.43	J/mol×K	806.11	Joback Method
cpg	555.64	J/mol×K	848.12	Joback Method
cpg	569.47	J/mol×K	890.13	Joback Method
cpg	600.41	J/mol×K	974.16	Joback Method

pvap	2.63e-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=R502493&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