Tris(p-chlorophenyl) borate

Other names: tris(4-chlorophenoxy)borane
Inchi: InChI=1S/C18H12BCl3O3/c20-13-1-7-16(8-2-13)23-19(24-17-9-3-14(21)4-10-17)25-18-11-5-15(22)6-12-18
InchiKey: JOAZIIBFQMIXJM-UHFFFAOYSA-N
Formula: C18H12BCl3O3
SMILES: Clc1ccc(OB(Oc2ccc(Cl)cc2)Oc2ccc(Cl)cc2)cc1
Mol. weight [g/mol]: 393.46
CAS: 7359-58-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.18		Crippen Method
logp	6.168		Crippen Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	30.60 ± 0.90	kJ/mol	452.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7359582&Units=SI

Legend

hvapt: Enthalpy of vaporization at a given temperature
log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient