

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)25-18-1
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/ci9903071
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

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