

2,4-Dibromophenyl bis(5-isopropyl-2-methylphenyl) phosphate

Inchi:	InChI=1S/C26H29Br2O4P/c1-16(2)20-9-7-18(5)25(13-20)31-33(29,30-24-12-11-22(27)1
InchiKey:	VIBSECJWMGAVHP-UHFFFAOYSA-N
Formula:	C26H29Br2O4P
SMILES:	Cc1ccc(C(C)C)cc1OP(=O)(Oc1cc(C(C)C)ccc1C)Oc1ccc(Br)cc1Br
Mol. weight [g/mol]:	596.29
CAS:	116295-53-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.78		Crippen Method
logp	9.720		Crippen Method
mcvol	384.860	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116295535&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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