

Phosphoric acid, octyl diphenyl ester

Other names:	Diphenyl octyl phosphate Disflamoll DPO Octyl diphenyl phosphate
Inchi:	InChI=1S/C20H27O4P/c1-2-3-4-5-6-13-18-22-25(21,23-19-14-9-7-10-15-19)24-20-16-11
InchiKey:	YAFOVCNAQTZDQB-UHFFFAOYSA-N
Formula:	C20H27O4P
SMILES:	CCCCCCCCOP(=O)(Oc1ccccc1)Oc1ccccc1
Mol. weight [g/mol]:	362.40
CAS:	115-88-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.22		Crippen Method
logp	6.630		Crippen Method
mcvol	289.080	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C115888&Units=SI

Legend

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

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