

Phosphonic diamide, n,n'-bis (p-butyl phenyl)-

Inchi:	InChI=1S/C20H29N2OP/c1-3-5-7-17-9-13-19(14-10-17)21-24(23)22-20-15-11-18(12-16-
InchiKey:	DZQFRORSEMPBNC-UHFFFAOYSA-N
Formula:	C20H29N2OP
SMILES:	CCCCc1ccc(N[PH](=O)Nc2ccc(CCCC)cc2)cc1
Mol. weight [g/mol]:	344.43
CAS:	116401-80-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.04		Crippen Method
logp	6.286		Crippen Method
mcvol	291.430	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=C116401800&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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