

Phosphoric acid, dibenzyl n,n-dimethyl carbamyl ester

Inchi: InChI=1S/C17H20NO5P/c1-18(2)17(19)23-24(20,21-13-15-9-5-3-6-10-15)22-14-16-11-7
InchiKey: YPTVJILMWZUUQT-UHFFFAOYSA-N
Formula: C17H20NO5P
SMILES: CN(C)C(=O)OP(=O)(OCc1ccccc1)OCc1ccccc1
Mol. weight [g/mol]: 349.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.98		Crippen Method
logp	4.226		Crippen Method
mcvol	258.360	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=B6009897&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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