

Phosphonic acid, (carbamoylmethyl)-, dibenzyl ester

Inchi: InChI=1S/C16H18NO4P/c17-16(18)13-22(19,20-11-14-7-3-1-4-8-14)21-12-15-9-5-2-6-10
InchiKey: MLSSAYAOIBJWSS-UHFFFAOYSA-N
Formula: C16H18NO4P
SMILES: N=C(O)CP(=O)(OCc1ccccc1)OCc1ccccc1
Mol. weight [g/mol]: 319.29
CAS: 101288-23-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.90		Crippen Method
logp	4.148		Crippen Method
mcvol	238.400	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=C101288237&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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