Dimethyl 3-nitro-phenyl phosphate

Inchi: InChI=1S/C8H10NO6P/c1-13-16(12,14-2)15-8-5-3-4-7(6-8)9(10)11/h3-6H,1-2H3
InchiKey: WVAUFDIKPLFXQL-UHFFFAOYSA-N
Formula: C8H10NO6P
SMILES: COP(=O)(OC)Oc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 247.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.10		Crippen Method
logp	2.374		Crippen Method
mcvol	161.180	ml/mol	McGowan Method
rinpol	1795.00		NIST Webbook
rinpol	1795.00		NIST Webbook
ripol	2720.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R169001&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol: Non-polar retention indices
ripol: Polar retention indices

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