

Dibutyl 3-nitro-phenyl phosphate

Inchi: InChI=1S/C14H22NO6P/c1-3-5-10-19-22(18,20-11-6-4-2)21-14-9-7-8-13(12-14)15(16)17
InchiKey: QDLDODXSBVDDJI-UHFFFAOYSA-N
Formula: C14H22NO6P
SMILES: CCCCOP(=O)(OCCCC)Oc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 331.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.61		Crippen Method
logp	4.715		Crippen Method
mcvol	245.720	ml/mol	McGowan Method
rinpol	2326.00		NIST Webbook
rinpol	2326.00		NIST Webbook
ripol	3112.00		NIST Webbook

Sources

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=R168840&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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