

Dibutyl 4-cyano-phenyl phosphate

Inchi: InChI=1S/C15H22NO4P/c1-3-5-11-18-21(17,19-12-6-4-2)20-15-9-7-14(13-16)8-10-15/h7
InchiKey: BDOCTTSTDBCLIQ-UHFFFAOYSA-N
Formula: C15H22NO4P
SMILES: CCCCOP(=O)(OCCCC)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 311.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.31		Crippen Method
logp	4.679		Crippen Method
mcvol	243.770	ml/mol	McGowan Method
rinpol	2228.00		NIST Webbook
rinpol	2228.00		NIST Webbook
ripol	3020.00		NIST Webbook
ripol	3020.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R168875&Units=SI>
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>

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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