

Dibutyl 3-cyano-phenyl phosphate

Inchi: InChI=1S/C15H22NO4P/c1-3-5-10-18-21(17,19-11-6-4-2)20-15-9-7-8-14(12-15)13-16/h7
InchiKey: VEZOQVJSNQWZGG-UHFFFAOYSA-N
Formula: C15H22NO4P
SMILES: CCCCOP(=O)(OCCCC)Oc1cccc(C#N)c1
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	2215.00		NIST Webbook
ripol	2989.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R168820&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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<https://www.chemeo.com/cid/31-069-1/Dibutyl-3-cyano-phenyl-phosphate.pdf>

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