

Diethyl,3-nitrophenyl phosphate

Inchi: InChI=1S/C10H14NO6P/c1-3-15-18(14,16-4-2)17-10-7-5-6-9(8-10)11(12)13/h5-8H,3-4H2
InchiKey: VXPBWHFHQQMMHT-UHFFFAOYSA-N
Formula: C10H14NO6P
SMILES: CCOP(=O)(OCC)Oc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 275.19
CAS: 4532-06-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.94		Crippen Method
logp	3.155		Crippen Method
mcvol	189.360	ml/mol	McGowan Method
rinpol	1880.00		NIST Webbook
ripol	2820.00		NIST Webbook
ripol	2820.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C4532063&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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