

(p-Chloro-Benzoyl)-phosphonic acid dimethyl ester

Inchi: InChI=1S/C9H10ClO4P/c1-13-15(12,14-2)9(11)7-3-5-8(10)6-4-7/h3-6H,1-2H3
InchiKey: TUKCAVDKGXMEKW-UHFFFAOYSA-N
Formula: C9H10ClO4P
SMILES: COP(=O)(OC)C(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 248.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.18		Crippen Method
logp	2.966		Crippen Method
mcvol	165.790	ml/mol	McGowan Method
rinpol	1716.00		NIST Webbook
rinpol	1729.00		NIST Webbook
rinpol	1716.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R205246&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/19-044-2/p-Chloro-Benzoyl-phosphonic-acid-dimethyl-ester.pdf>

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