Tetraethyl dimethylaminomethylenediphosphonate

Other names: Phosphonic acid, [(dimethylamino)methylene]bis-, tetraethyl ester
tetraethyl [(dimethylamino)methylene]bisphosphonate
Inchi: InChI=1S/C11H27NO6P2/c1-7-15-19(13,16-8-2)11(12(5)6)20(14,17-9-3)18-10-4/h11H,7-
InchiKey: SQDDGOVNJMIFFT-UHFFFAOYSA-N
Formula: C11H27NO6P2
SMILES: CCOP(=O)(OCC)C(N(C)C)P(=O)(OCC)OCC
Mol. weight [g/mol]: 331.28
CAS: 18855-52-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.00		Crippen Method
logp	3.364		Crippen Method
mcvol	251.970	ml/mol	McGowan Method

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=C18855522&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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