

di-t-Butyl phosphite

Other names:	di-tert-Butyl phosphite Phosphonic acid, bis(1,1-dimethylethyl) ester Di-tert-butyl hydrogen phosphate bis(1,1-dimethylethyl) phosphonate
Inchi:	InChI=1S/C8H19O3P/c1-7(2,3)10-12(9)11-8(4,5)6/h9H,1-6H3
InchiKey:	RRJHOMPUEYYASJ-UHFFFAOYSA-N
Formula:	C8H19O3P
SMILES:	CC(C)(C)OP(O)OC(C)(C)C
Mol. weight [g/mol]:	194.21
CAS:	13086-84-5

Physical Properties

Property code	Value	Unit	Source
log10ws	0.34		Crippen Method
logp	2.836		Crippen Method
mcvol	161.650	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13086845&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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