

Cyclo-tris(dimethoxyphosphonitrile)

Inchi:	InChI=1S/C6H18N3O6P3/c1-10-16(11-2)7-17(12-3,13-4)9-18(8-16,14-5)15-6/h1-6H3
InchiKey:	CNQBXJDCTHCEFG-UHFFFAOYSA-N
Formula:	C6H18N3O6P3
SMILES:	COP1(OC)=NP(OC)(OC)=NP(OC)(OC)=N1
Mol. weight [g/mol]:	321.14
CAS:	957-13-1

Physical Properties

Property code	Value	Unit	Source
log10ws	7.72		Crippen Method
logp	3.717		Crippen Method
mcvol	211.080	ml/mol	McGowan Method

Sources

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=C957131&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/96-792-7/Cyclo-tris-dimethoxyphosphonitrile.pdf>

Generated by Cheméo on 2024-05-17 03:33:28.837793795 +0000 UTC m=+18206057.758371106.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.