Diphosphine, tetrakis(trifluoromethyl)-

Other names:	Diphosphine, tetrakis(trifluoromethyl)-, gauche conformer Diphosphine, tetrakis(trifluoromethyl)-, trans conformer (Tetra-kis-trifluoromethyl)diphosphine
Inchi:	InChI=1S/C4F12P2/c5-1(6,7)17(2(8,9)10)18(3(11,12)13)4(14,15)16
InchiKey:	GFWZGKUMKFSQHH-UHFFFAOYSA-N
Formula:	C4F12P2
SMILES:	FC(F)(F)P(P(C(F)(F)F)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]:	337.97
CAS:	2714-60-5

Physical Properties

Property code	Value	Unit	Source
ie	10.71	eV	NIST Webbook
ie	10.71	eV	NIST Webbook
ie	11.57	eV	NIST Webbook
log10ws	1.17		Crippen Method
logp	5.944		Crippen Method
mcvol	129.380	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2714605&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

ie:	Ionization energy
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/87-941-1/Diphosphine-tetrakis-trifluoromethyl.pdf

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