

Phosphine, bis(trifluoromethyl)-

Other names:	Bis(trifluoromethyl)phosphine
Inchi:	InChI=1S/C2HF6P/c3-1(4,5)9-2(6,7)8/h9H
InchiKey:	CJOZYRZUMSWLHJ-UHFFFAOYSA-N
Formula:	C2HF6P
SMILES:	FC(F)(F)PC(F)(F)F
Mol. weight [g/mol]:	169.99
CAS:	460-96-8

Physical Properties

Property code	Value	Unit	Source
ie	11.50	eV	NIST Webbook
ie	11.51	eV	NIST Webbook
log10ws	0.98		Crippen Method
logp	2.705		Crippen Method
mcvol	70.120	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=C460968&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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