

Sarin

Other names:	O-Isopropyl methylphosphonofluoridate Phosphonofluoridic acid, methyl-, 1-methylethyl ester Phosphonofluoridic acid, methyl-, isopropyl ester GB Isopropoxymethylphosphoryl fluoride Isopropyl methylfluorophosphonate Isopropyl methylphosphonofluoridate Methylfluorophosphoric acid isopropyl ester Methylphosphonofluoridic acid isopropyl ester O-Isopropyl methylfluorophosphonate Zarin EA 1208 IMPF Isopropylester kyseliny methylfluorofosfonove Isopropyl methanefluorophosphonate Isopropyl methylfluorophosphate Isopropyl-methyl-phosphoryl fluoride Methylfluorophosphorsaeureisopropyl ester Methylphosphonofluoridic acid 1-methylethyl ester MFI Phosphine oxide, fluoroisopropoxymethyl- Phosphoric acid, methylfluoro-, isopropyl ester Sarin II T-144 T-2106 TL 1618 Trilone 46 1-Methylethyl methylphosphonofluoridate Phosphonofluoridic acid, P-methyl-, 1-methylethyl ester (.+/-)-Sarin
Inchi:	InChI=1S/C4H10FO2P/c1-4(2)7-8(3,5)6/h4H,1-3H3
InchiKey:	DYAHQFWOVKZOOW-UHFFFAOYSA-N
Formula:	C4H10FO2P
SMILES:	CC(C)OP(C)(=O)F
Mol. weight [g/mol]:	140.09
CAS:	107-44-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.82		Crippen Method
logp	2.204		Crippen Method
mcvol	101.190	ml/mol	McGowan Method
rinpol	820.00		NIST Webbook
rinpol	817.00		NIST Webbook
rinpol	824.00		NIST Webbook
rinpol	792.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	818.37		NIST Webbook
rinpol	819.25		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	817.00		NIST Webbook
rinpol	791.80		NIST Webbook
rinpol	823.80		NIST Webbook
rinpol	820.20		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	789.00		NIST Webbook
ripol	1297.00		NIST Webbook
ripol	1297.00		NIST Webbook
ripol	1278.40		NIST Webbook

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=C107448&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

rinpol: Non-polar retention indices

ripol: Polar retention indices

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