

Soman

Other names:	Phosphonofluoridic acid, methyl-, 1,2,2-trimethylpropyl ester 1,2,2-Trimethylpropoxyfluorophosphine oxide O-Pinacolyl methylphosphonofluoridate GD Methyl pinacolyl phosphonofluoridate Methyl pinacolylphosphoryl fluoride Phosphine oxide, fluoromethyl(1,2,2-trimethylpropoxy)- Pinacoloxymethylphosphoryl fluoride Pinacolyl methylfluorophosphonate Pinacolyl methylphosphonofluoridate PMFP Zoman 1,2,2-Trimethylpropyl methylphosphonofluoridate 3,3-Dimethyl-n-but-2-yl methylphosphonofluoridate Methylphosphonofluoridic acid 1,2,2-trimethylpropyl ester Soman # 1 Soman # 2 Pinacolyl methylphosphonofluoridate, diastereomer # 1 Pinacolyl methylphosphonofluoridate, diastereomer # 2
Inchi:	InChI=1S/C7H16FO2P/c1-6(7(2,3)4)10-11(5,8)9/h6H,1-5H3
InchiKey:	GRXKLBBBQUKJJZ-UHFFFAOYSA-N
Formula:	C7H16FO2P
SMILES:	CC(OP(C)(=O)F)C(C)(C)C
Mol. weight [g/mol]:	182.17
CAS:	96-64-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.84		Crippen Method
logp	3.230		Crippen Method
mcvol	143.460	ml/mol	McGowan Method
rinpol	1016.00		NIST Webbook
rinpol	1039.71		NIST Webbook
rinpol	1040.99		NIST Webbook
rinpol	1044.07		NIST Webbook
rinpol	1045.44		NIST Webbook
rinpol	1012.00		NIST Webbook

rinpol	1016.00	NIST Webbook
rinpol	1038.00	NIST Webbook
rinpol	1016.00	NIST Webbook
rinpol	1008.10	NIST Webbook
rinpol	1012.90	NIST Webbook
rinpol	1045.20	NIST Webbook
rinpol	1049.30	NIST Webbook
rinpol	1043.70	NIST Webbook
rinpol	1045.00	NIST Webbook
rinpol	1012.00	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1038.00	NIST Webbook
rinpol	1043.00	NIST Webbook
rinpol	1042.00	NIST Webbook
rinpol	1047.00	NIST Webbook
rinpol	1044.00	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1044.00	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1008.00	NIST Webbook
rinpol	1040.99	NIST Webbook
rinpol	1038.00	NIST Webbook
rinpol	1049.30	NIST Webbook
rinpol	1044.00	NIST Webbook
rinpol	1013.00	NIST Webbook
rinpol	1008.00	NIST Webbook
ripol	1478.00	NIST Webbook
ripol	1490.00	NIST Webbook
ripol	1478.00	NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C96640&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

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

Latest version available from:

<https://www.chemeo.com/cid/33-471-2/Soman.pdf>

Generated by Cheméo on 2024-04-26 06:29:12.925503245 +0000 UTC m=+16402201.846080557.

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