

n-Butyl methylphosphonofluoridate

Other names:	Phosphonofluoridic acid, methyl-, butyl ester Methylphoshonic acid, fluoroanhydride-, butyl ester Butyl methylphosphonofluoridate
Inchi:	InChI=1S/C5H12FO2P/c1-3-4-5-8-9(2,6)7/h3-5H2,1-2H3
InchiKey:	DPBYNDKWLKHTAK-UHFFFAOYSA-N
Formula:	C5H12FO2P
SMILES:	CCCCOP(C)(=O)F
Mol. weight [g/mol]:	154.12
CAS:	352-63-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.13		Crippen Method
logp	2.595		Crippen Method
mcvol	115.280	ml/mol	McGowan Method
rinpol	971.00		NIST Webbook
rinpol	971.20		NIST Webbook
rinpol	971.00		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=C352636&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

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

rinpol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/43-336-1/n-Butyl-methylphosphonofluoridate.pdf>

Generated by Cheméo on 2025-12-05 08:27:13.789127993 +0000 UTC m=+4671431.319168656.

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