

Tabun

Other names:	O-Ethyl N,N-dimethyl phosphoramidocyanidate GA Phosphoramidocyanidic acid, dimethyl-, ethyl ester Dimethylamidoethoxyphosphoryl cyanide Ethyl dimethylamidocyanophosphate Ethyl dimethylphosphoramidocyanidate Dimethylaminocyanphosphorsaeureaethylester Dimethylphosphoramidocyanidic acid, ethyl ester EA 1205 Ethyl N,N-dimethylphosphoramidocyanidate Ethyl N,N-dimethylamino cyanophosphate Ethylester-dimethylamid kyseliny kyanfosfonove Gelan I Le-100 T-2104 TL 1578 Taboon A Trilon 83 GA (chemical warfare agent) Phosphoramidocyanidic acid, N,N-dimethyl-, ethyl ester
Inchi:	InChI=1S/C5H11N2O2P/c1-4-9-10(8,5-6)7(2)3/h4H2,1-3H3
InchiKey:	PJVJTCIRVMBVIA-UHFFFAOYSA-N
Formula:	C5H11N2O2P
SMILES:	CCOP(=O)(C#N)N(C)C
Mol. weight [g/mol]:	162.13
CAS:	77-81-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.21		Crippen Method
logp	1.259		Crippen Method
mcvol	124.870	ml/mol	McGowan Method
rinpol	1131.00		NIST Webbook
rinpol	1133.00		NIST Webbook
ripol	1790.40		NIST Webbook
ripol	1790.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77816&Units=SI

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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