Phosphorylethanolamine

Other names:	2-Aminoethyl dihydrogen phosphate O-Phosphocolamine O-Phosphoethanolamine Colaminphosphoric acid O-Phosphorylethanolamine Ethanol, 2-amino-, dihydrogen phosphate Colamine phosphate Ethanol, 2-amino-, dihydrogen phosphate (ester) Ethanol, 2-amino-, phosphate Ethanolamine phosphate Ethanolamine O-phosphate Mono(2-aminoethyl) phosphate Pe 104 Phosphoethanolamine Phosphonoethanolamine Phosphoryethanolamine Ethanol, 2-amino-, 1-(dihydrogen phosphate) NSC 254167
Inchi:	InChI=1S/C2H8NO4P/c3-1-2-7-8(4,5)6/h1-3H2,(H2,4,5,6)
InchiKey:	SUHOOTKUPISOBE-UHFFFAOYSA-N
Formula:	C2H8NO4P
SMILES:	NCCOP(=O)(O)O
Mol. weight [g/mol]:	141.06
CAS:	1071-23-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.97		Crippen Method
logp	-0.946		Crippen Method
mcvol	92.960	ml/mol	McGowan Method

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=C1071234&Units=SI

Legend

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

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https://www.chemeo.com/cid/88-192-2/Phosphorylethanolamine.pdf

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