

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: | SUH00TKUPISOBE-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

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1071234&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

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

Generated by Cheméo on 2024-04-24 03:37:17.704115115 +0000 UTC m=+16219086.624692442.

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