# 2-Propanol, 1,3-dibromo-, phosphate (3:1)

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|---|---|
| **Other names:** | Tris(1,3-dibromo-2-propyl)phosphate |
| | Tris(1-bromomethyl-2-bromoethyl)phosphate |
| **Inchi:** | InChI=1S/C9H15Br6O4P/c10-1-7(2-11)17-20(16,18-8(3-12)4-13)19-9(5-14)6-15/h7-9H,1 |
| **InchiKey:** | RZEYUZWXPABTCN-UHFFFAOYSA-N |
| **Formula:** | C9H15Br6O4P |
| **SMILES:** | O=P(OC(CBr)CBr)(OC(CBr)CBr)OC(CBr)CBr |
| **Mol. weight [g/mol]:** | 697.61 |
| **CAS:** | 18713-51-4 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -7.04 | | Crippen Method |
| logp | 5.620 | | Crippen Method |
| mcvol | 286.610 | ml/mol | McGowan Method |

## Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C18713514&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

## Legend

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

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