Phosphonic acid, ethyl-, ethyl ester, diester wtih 1,4-butanediol

Inchi: InChI=1S/C12H28O6P2/c1-5-15-19(13,7-3)17-11-9-10-12-18-20(14,8-4)16-6-2/h5-12H2,
InchiKey: QHXHEDUSWYCAHZ-UHFFFAOYSA-N
Formula: C12H28O6P2
SMILES: CCOP(=O)(CC)OCCCCOP(=O)(CC)OCC
Mol. weight [g/mol]: 330.29
CAS: 5284-05-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.74		Crippen Method
logp	4.299		Crippen Method
mcvol	256.080	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=C5284059&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