

Phosphonic acid, ethyl-, ethyl ester, diester with 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/ci9903071
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/91-166-7/Phosphonic-acid-ethyl-ethyl-ester-diester-with-1-4-butanediol.pdf>

Generated by Cheméo on 2024-04-20 12:51:50.423178068 +0000 UTC m=+15906759.343755379.

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