

Dibutyl butanephosphonate

Other names:	Di-n-butyl n-butylphosphonate Dibutylbutylphosphonate dibutyl butylphosphonate phosphonic acid, butyl-, dibutyl ester
Inchi:	InChI=1S/C12H27O3P/c1-4-7-10-14-16(13,12-9-6-3)15-11-8-5-2/h4-12H2,1-3H3
InchiKey:	JPGXOMADPRULAC-UHFFFAOYSA-N
Formula:	C12H27O3P
SMILES:	CCCCOP(=O)(CCCC)OCCCC
Mol. weight [g/mol]:	250.31
CAS:	78-46-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.29		Crippen Method
logp	4.613		Crippen Method
mvol	218.010	ml/mol	McGowan Method
tb	566.07	K	Correlation of normal boiling points of dialkylalkyl phosphonates with topological indices on the gas chromatographic retention data

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of dialkylalkyl phosphonates in supercritical carbon dioxide:	https://www.doi.org/10.1016/j.fluid.2016.12.011
Correlation of normal boiling points of dialkylalkyl phosphonates with topological indices on the gas chromatographic retention data:	https://www.doi.org/10.1016/j.tca.2014.11.027
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78466&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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