

Dibutyl benzylphosphonate

Other names:	Phosphonic acid, benzyl-, dibutyl ester Benzylphosphonic acid dibutyl ester Di-n-butyl benzylphosphonate Dibutoxyphosphorylmethylbenzene
Inchi:	InChI=1S/C15H25O3P/c1-3-5-12-17-19(16,18-13-6-4-2)14-15-10-8-7-9-11-15/h7-11H,3-
InchiKey:	ARIYRPOBFJRCEU-UHFFFAOYSA-N
Formula:	C15H25O3P
SMILES:	CCCCOP(=O)(Cc1ccccc1)OCCCC
Mol. weight [g/mol]:	284.33
CAS:	3762-27-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.15		Crippen Method
logp	5.013		Crippen Method
mcvol	236.520	ml/mol	McGowan Method
rinpol	1985.00		NIST Webbook
rinpol	1985.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	414.50 ± 1.50	K	0.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3762274&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tbrp:	Boiling point at reduced pressure

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