

5'-Inosinic acid, dibutyl ester

Inchi:	InChI=1S/C18H29N4O8P/c1-3-5-7-27-31(26,28-8-6-4-2)29-9-12-14(23)15(24)18(30-12)2
InchiKey:	KQONLLMXDCOJTN-UHFFFAOYSA-N
Formula:	C18H29N4O8P
SMILES:	CCCCOP(=O)(OCCCC)OCC1OC(n2cnc3c(=O)[nH]cnc32)C(O)C1O
Mol. weight [g/mol]:	460.42
CAS:	15923-57-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.14		Crippen Method
logp	1.015		Crippen Method
mcvol	322.040	ml/mol	McGowan Method

Sources

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=C15923576&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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