

Uracil, 1,3-bis(p-nitrobenzyl)-

Inchi:	InChI=1S/C18H14N4O6/c23-17-9-10-19(11-13-1-5-15(6-2-13)21(25)26)18(24)20(17)12-
InchiKey:	YZAFQHMMBCUUPR-UHFFFAOYSA-N
Formula:	C18H14N4O6
SMILES:	O=c1ccn(Cc2ccc([N+](=O)[O-])cc2)c(=O)n1Cc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	382.33
CAS:	116496-70-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.74		Crippen Method
logp	1.923		Crippen Method
mcvol	259.740	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C116496709&Units=SI

Legend

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

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