

9-Hydroxy-9-(2'-pyridyl)-xanthene

Inchi:	InChI=1S/C18H13NO2/c20-18(17-11-5-6-12-19-17)13-7-1-3-9-15(13)21-16-10-4-2-8-14(
InchiKey:	DZUKNWFAOPXQIV-UHFFFAOYSA-N
Formula:	C18H13NO2
SMILES:	OC1(c2ccccc2)c2ccccc2Oc2ccccc21
Mol. weight [g/mol]:	275.30
CAS:	67916-68-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.37		Crippen Method
logp	3.471		Crippen Method
mcvol	204.060	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=C67916681&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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