

1,2-Ethanediol, 1,2-bis(6-methylpyridyl)-

Other names:	1,2-bis(6-methyl-2-pyridyl)ethanediol
Inchi:	InChI=1S/C14H16N2O2/c1-9-5-3-7-11(15-9)13(17)14(18)12-8-4-6-10(2)16-12/h3-8,13-14
InchiKey:	BQACYHPDFUQUVCV-UHFFFAOYSA-N
Formula:	C14H16N2O2
SMILES:	Cc1cccc(C(O)C(O)c2cccc(C)n2)n1
Mol. weight [g/mol]:	244.29
CAS:	6630-20-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.82		Crippen Method
logp	1.860		Crippen Method
mcvol	192.300	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6630202&Units=SI
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

Legend

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

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