

PIPEROXAN

Other names:	1,4-Benzodioxane, 2-(piperidinomethyl)- 2-Piperidinomethyl-1,4-benzodioxan 2-Piperidinomethyl-1,4-benzodioxane 933F Benodaine F933 Fourneau 933 Piperidine, 1-((2,3-dihydro-1,4-benzodioxin-2-yl)methyl)- Piperidine, 1-(1,4-benzodioxan-2-ylmethyl)- Piperoxane
Inchi:	InChI=1S/C14H19NO2/c1-4-8-15(9-5-1)10-12-11-16-13-6-2-3-7-14(13)17-12/h2-3,6-7,12
InchiKey:	LYKMMUBOEFYJQG-UHFFFAOYSA-N
Formula:	C14H19NO2
SMILES:	c1ccc2c(c1)OCC(CN1CCCCC1)O2
Mol. weight [g/mol]:	233.31

Physical Properties

Property code	Value	Unit	Source
logp	2.312		Crippen Method
mcvol	184.360	ml/mol	McGowan Method
rinpol	1840.00		NIST Webbook
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Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C59392&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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