

(E)-3-(Benzo[d][1,3]dioxol-5-yl)-1-(piperidin-1-yl)p

Inchi:	InChI=1S/C15H17NO3/c17-15(16-8-2-1-3-9-16)7-5-12-4-6-13-14(10-12)19-11-18-13/h4-
InchiKey:	BLPUOQGGBJPXRL-FNORWQNLSA-N
Formula:	C15H17NO3
SMILES:	O=C(C=Cc1ccc2c(c1)OCO2)N1CCCCC1
Mol. weight [g/mol]:	259.30
CAS:	82857-82-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.26		Crippen Method
logp	2.441		Crippen Method
mcvol	195.720	ml/mol	McGowan Method
rinpol	2558.60		NIST Webbook
rinpol	2506.00		NIST Webbook
rinpol	2506.00		NIST Webbook
rinpol	2558.60		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C82857827&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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