

(R)-1-Methoxy-6-methyl-5,6,6a,7-tetrahydro-4H-dibenz[de]quinolin-2-ol

Inchi:	InChI=1S/C18H19NO2/c1-19-8-7-12-10-15(20)18(21-2)17-13-6-4-3-5-11(13)9-14(19)16(20)
InchiKey:	AKXOIHNHFHOEPHN-CQSZACIVSA-N
Formula:	C18H19NO2
SMILES:	COc1c(O)cc2c3c1-c1ccccc1CC3N(C)CC2
Mol. weight [g/mol]:	281.35
CAS:	3153-55-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.55		Crippen Method
logp	3.153		Crippen Method
mcvol	216.960	ml/mol	McGowan Method
rinpol	2447.10		NIST Webbook
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Sources

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=C3153557&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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