

Racemethorphan

Other names:	Morphinan, 3-methoxy-17-methyl-, (.+/-.)- DL-3-Methoxy-N-methylmorphinan (.+/-.)-3-Methoxy-N-methylmorphinan (.+/-.)-3-Methoxy-17-methylmorphinan Deoxydihydrothebacodine 3-Methoxy-17-methylmorphinan
Inchi:	InChI=1S/C18H25NO/c1-19-10-9-18-8-4-3-5-15(18)17(19)11-13-6-7-14(20-2)12-16(13)1
InchiKey:	MKXZASYAUGDDCJ-UHFFFAOYSA-N
Formula:	C18H25NO
SMILES:	<chem>COc1ccc2c(c1)C13CCCCC1C(C2)N(C)CC3</chem>
Mol. weight [g/mol]:	271.40
CAS:	510-53-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.93		Crippen Method
logp	3.383		Crippen Method
mcvol	223.990	ml/mol	McGowan Method
rinpol	2129.00		NIST Webbook
rinpol	2124.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C510532&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rinpol: Non-polar retention indices

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