

Metazocine

Other names:	2,6-Methano-3-benzazocin-8-ol, 1,2,3,4,5,6-hexahydro-3,6,11-trimethyl-2'-Hydroxy-2,5,9-trimethyl-6,7-benzomorphan Methobenzmorphan
Inchi:	InChI=1S/C15H21NO/c1-10-14-8-11-4-5-12(17)9-13(11)15(10,2)6-7-16(14)3/h4-5,9-10,1
InchiKey:	YGSVZRIZCHZUHB-UHFFFAOYSA-N
Formula:	C15H21NO
SMILES:	<chem>CC1C2Cc3ccc(O)cc3C1(C)CCN2C</chem>
Mol. weight [g/mol]:	231.33
CAS:	3734-52-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.62		Crippen Method
logp	2.546		Crippen Method
mcvol	192.580	ml/mol	McGowan Method
rinpol	1920.00		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=C3734529&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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<https://www.chemeo.com/cid/82-750-8/Metazocine.pdf>

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