Thebaine

Other names:	Morphinan, 6,7,8,14-tetradehydro-4,5-epoxy-3,6-dimethoxy-17-methyl-, (5«alpha»)- Morphinan, 6,7,8,14-tetradehydro-4,5«alpha»-epoxy-3,6-dimethoxy-17-methyl- Paramorphine Tebain Thebain
Inchi:	InChI=1S/C19H21NO3/c1-20-9-8-19-12-5-7-15(22-3)18(19)23-17-14(21-2)6-4-11(16(17)
InchiKey:	FQXXSQDCDRQNQE-UHFFFAOYSA-N
Formula:	C19H21NO3
SMILES:	COC1=CC=C2C3Cc4ccc(OC)c5c4C2(CCN3C)C1O5
Mol. weight [g/mol]:	311.37
CAS:	115-37-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.58		Crippen Method
logp	2.425		Crippen Method
mcvol	230.360	ml/mol	McGowan Method
rinpol	2559.00		NIST Webbook
rinpol	2558.00		NIST Webbook
rinpol	2522.00		NIST Webbook
rinpol	2550.00		NIST Webbook
rinpol	2520.00		NIST Webbook
rinpol	2555.00		NIST Webbook
rinpol	2492.00		NIST Webbook
rinpol	2485.00		NIST Webbook
rinpol	2505.00		NIST Webbook
rinpol	2492.00		NIST Webbook
rinpol	2525.00		NIST Webbook
rinpol	2517.00		NIST Webbook
rinpol	2485.00		NIST Webbook
rinpol	2525.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C115377&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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