

Codeinone, 14-hydroxy-

Other names:	(5«alpha»)-7,8-didehydro-4,5-epoxy-14-hydroxy-3-methoxy-17-methylmorphinan-6-one
Inchi:	InChI=1S/C18H19NO4/c1-19-8-7-17-14-10-3-4-12(22-2)15(14)23-16(17)11(20)5-6-18(17)
InchiKey:	YYCRAERBSFHMPL-UHFFFAOYSA-N
Formula:	C18H19NO4
SMILES:	COc1ccc2c3c1OC1C(=O)C=CC4(O)C(C2)N(C)CCC314
Mol. weight [g/mol]:	313.35
CAS:	508-54-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.38		Crippen Method
logp	0.824		Crippen Method
mcvol	222.140	ml/mol	McGowan Method

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=C508543&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/99-254-1/Codeinone-14-hydroxy.pdf>

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