Apomorphine

Other names:	4H-Dibenzo[de,g]quinoline-10,11-diol, 5,6,6a,7-tetrahydro-6-methyl-, (R)- 6a-«beta»-Aporphine-10,11-diol Apomorfin Apormorphine 4H-Dibenzo(de,g)quinoline-10,11-diol, 5,6,6a,7-tetrahydro-6-methyl- 5,6,6a,7-Tetrahydro-6-methyl-4H-dibenzo[de,g]quinolin-10,11-diol
Inchi:	InChI=1S/C17H17NO2/c1-18-8-7-10-3-2-4-12-15(10)13(18)9-11-5-6-14(19)17(20)16(11)...
InchiKey:	VMWNQDUVQKEIOC-UHFFFAOYSA-N
Formula:	C17H17NO2
SMILES:	CN1CCc2cccc3c2C1Cc1ccc(O)c(O)c1-3
Mol. weight [g/mol]:	267.32
CAS:	58-00-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.98		Crippen Method
logp	2.850		Crippen Method
mcvol	202.870	ml/mol	McGowan Method
rinpol	2530.00		NIST Webbook
rinpol	2530.00		NIST Webbook
rinpol	2530.00		NIST Webbook

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=C58004&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices