

Vobassan-17-oic acid, 4-demethyl-3-oxo-, methyl ester

Other names:	Perivin Perivine
Inchi:	InChI=1S/C20H22N2O3/c1-3-11-10-21-16-8-14-12-6-4-5-7-15(12)22-19(14)17(23)9-13(1)
InchiKey:	NKTORRNHKYVXSU-QDEBKDIKSA-N
Formula:	C20H22N2O3
SMILES:	CC=C1CNC2Cc3c([nH]c4cccc34)C(=O)CC1C2C(=O)OC
Mol. weight [g/mol]:	338.40
CAS:	2673-40-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.63		Crippen Method
logp	2.138		Crippen Method
mcvol	256.690	ml/mol	McGowan Method

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=C2673407&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i

Legend

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

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