

Perindopril desethyl - H2) Me (Perindoprilate - H2O Me)

Inchi:	InChI=1S/C18H28N2O4/c1-4-7-14(18(23)24-3)19-11(2)16(21)20-13-9-6-5-8-12(13)10-15
InchiKey:	RYNZKGIBSLIAFS-MFTHNPBUSA-N
Formula:	C18H28N2O4
SMILES:	CCCC(C(=O)OC)N1C(=O)C2CC3CCCCC3N2C(=O)C1C
Mol. weight [g/mol]:	336.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.80		Crippen Method
logp	1.719		Crippen Method
mcvol	262.440	ml/mol	McGowan Method
rinsol	2560.00		NIST Webbook

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=R549932&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
rinsol:	Non-polar retention indices

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<https://www.chemeo.com/cid/68-187-0/Perindopril-desethyl-H2-Me-Perindoprilate-H2O-Me.pdf>

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