

Cyclopentyl-hydroxy-phenyl-acetic acid 1-methyl-pyrrolidin-3-yl ester

Inchi: InChI=1S/C18H25NO3/c1-19-12-11-16(13-19)22-17(20)18(21,15-9-5-6-10-15)14-7-3-2-4
InchiKey: OVGMPKPGXRHJNKJ-UHFFFAOYSA-N
Formula: C18H25NO3
SMILES: CN1CCC(OC(=O)C(O)(c2ccccc2)C2CCCC2)C1
Mol. weight [g/mol]: 303.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.98		Crippen Method
logp	2.312		Crippen Method
mcvol	242.290	ml/mol	McGowan Method
rinpol	2120.00		NIST Webbook
rinpol	2120.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R489246&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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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