

Ipanguline B1

Inchi: InChI=1S/C20H27NO7/c1-12(22)20(2,26)19(25)27-11-13-7-9-21-10-8-16(17(13)21)28-18
InchiKey: HQNBAGWQDKKAMY-TZLBMGJLSA-N
Formula: C20H27NO7
SMILES: CC(O)C(C)(O)C(=O)OCC1CCN2CCC(OC(=O)c3ccccc3O)C12
Mol. weight [g/mol]: 393.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.24		Crippen Method
logp	0.687		Crippen Method
mcvol	289.650	ml/mol	McGowan Method
rinpol	2772.00		NIST Webbook
rinpol	2772.00		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=R394871&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
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/19-848-0/Ipanguline-B1.pdf>

Generated by Cheméo on 2025-12-05 19:53:58.429943797 +0000 UTC m=+4712635.959984467.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.