Ipanguline C2

Inchi: InChI=1S/C20H33NO7/c1-6-12(2)18(23)28-16-8-10-21-9-7-15(17(16)21)11-26-19(24)20(
InchiKey: QSDVUZIHMDWHEK-SRMJLOKFSA-N
Formula: C20H33NO7
SMILES: CCC(C)C(=O)OC1CCN2CCC(COC(=O)C(C)(O)C(C)OC(C)=O)C12
Mol. weight [g/mol]: 399.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Crippen Method
logp	1.284		Crippen Method
mcvol	309.110	ml/mol	McGowan Method
rinpol	2426.00		NIST Webbook
rinpol	2426.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R394915&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.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

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