

Isoipanguline 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: QSDVUZHMDWHEK-UULZSWRBSA-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	2391.00		NIST Webbook
rinpol	2391.00		NIST Webbook
rinpol	2391.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R395205&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

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<https://www.chemeo.com/cid/49-139-4/Isoipanguline-C2.pdf>

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