Ipanguline D3

Inchi:	InChI=1S/C13H23NO5/c1-8(15)13(2,18)12(17)19-7-9-3-5-14-6-4-10(16)11(9)14/h8-11,15
InchiKey:	GWTMMYYKPSYPDW-LFEBVRLFSA-N
Formula:	C13H23NO5
SMILES:	CC(O)C(C)(O)C(=O)OCC1CCN2CCC(O)C12
Mol. weight [g/mol]:	273.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.48		Crippen Method
logp	-0.883		Crippen Method
mcvol	207.340	ml/mol	McGowan Method
rinpol	2037.00		NIST Webbook
rinpol	2037.00		NIST Webbook
rinpol	2037.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R395012&Units=SI

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/60-837-6/Ipanguline-D3.pdf

Generated by Cheméo on 2024-10-12 05:14:20.230404143 +0000 UTC m=+3290922.867373392.

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