Ipanguline D6

Inchi: InChI=1S/C16H21NO3/c18-11-13-6-8-17-9-7-14(16(13)17)20-15(19)10-12-4-2-1-3-5-12/l
InchiKey: SAFDSKJGKYBCKH-UIDSBSESSA-N
Formula: C16H21NO3
SMILES: O=C(Cc1ccccc1)OC1CCN2CCC(CO)C12
Mol. weight [g/mol]: 275.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.09		Crippen Method
logp	1.227		Crippen Method
mcvol	214.110	ml/mol	McGowan Method
rinpol	2168.00		NIST Webbook
rinpol	2168.00		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=R394811&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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