

Sultopride

Inchi: InChI=1S/C17H26N2O4S/c1-4-19-10-6-7-13(19)12-18-17(20)15-11-14(24(21,22)5-2)8-9
InchiKey: UNRHXEPRDKXPRTM-UHFFFAOYSA-N
Formula: C17H26N2O4S
SMILES: CCN1CCCC1CNC(=O)c1cc(S(=O)(=O)CC)ccc1OC
Mol. weight [g/mol]: 354.46
CAS: 53583-79-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.14		Crippen Method
logp	1.703		Crippen Method
mcvol	271.260	ml/mol	McGowan Method
rinpol	3065.00		NIST Webbook
rinpol	3065.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C53583792&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

Latest version available from:

<https://www.chemeo.com/cid/111-507-5/Sultopride.pdf>

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