Fenspiride

Other names: 8-(2-phenylethyl)-1-oxa-3,8-diazaspiro[4.5]decan-2-one hydrochloride
Inchi: InChI=1S/C15H20N2O2/c18-14-16-12-15(19-14)7-10-17(11-8-15)9-6-13-4-2-1-3-5-13/h1
InchiKey: FVNFBBAOMBJTST-UHFFFAOYSA-N
Formula: C15H20N2O2
SMILES: O=C1NCC2(CCN(CCc3ccccc3)CC2)O1
Mol. weight [g/mol]: 260.33
CAS: 5053-08-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.71		Crippen Method
logp	1.803		Crippen Method
mcvol	204.130	ml/mol	McGowan Method
rinpol	2530.00		NIST Webbook
rinpol	2530.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5053087&Units=SI
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

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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