2-(7,8-Dioxa-bicyclo[4.2.0]octa-1,3,5-trien-3-yl)-7-e

Inchi: InChI=1S/C20H20O3/c1-4-6-13-9-14(5-2)20-16(10-13)12(3)19(21-20)15-7-8-17-18(11-15

InchiKey: SYHONOFWMGINBI-UHFFFAOYSA-N

Formula: C20H20O3

SMILES: C=CCc1cc(CC)c2c(c1)C(C)C(c1ccc3ooc3c1)O2

Mol. weight [g/mol]: 308.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-15.48		Crippen Method
logp	5.554		Crippen Method
mcvol	236.730	ml/mol	McGowan Method
rinpol	2623.00		NIST Webbook
rinpol	2623.00		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=R294305&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

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