Oxatomide

Inchi: InChI=1S/C27H30N4O/c32-27-28-24-14-7-8-15-25(24)31(27)17-9-16-29-18-20-30(21-19
InchiKey: BAINIUMDFURPJM-UHFFFAOYSA-N
Formula: C27H30N4O
SMILES: O=c1[nH]c2ccccc2n1CCCN1CCN(C(c2ccccc2)c2ccccc2)CC1
Mol. weight [g/mol]: 426.55
CAS: 60607-34-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.52		Crippen Method
logp	3.645		Crippen Method
mcvol	339.780	ml/mol	McGowan Method
rinpol	3200.00		NIST Webbook
rinpol	3200.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C60607343&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