

# 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
rinpola	3200.00		NIST Webbook
rinpola	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](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  
**rinpola:** Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/48-975-7/Oxatomide.pdf>

Generated by Cheméo on 2024-04-29 00:31:47.880816127 +0000 UTC m=+16639956.801393443.

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