

# Letrozole

<b>Other names:</b>	Femara
<b>Inchi:</b>	InChI=1S/C17H11N5/c18-9-13-1-5-15(6-2-13)17(22-12-20-11-21-22)16-7-3-14(10-19)4-8
<b>InchiKey:</b>	HPJKCIUCZWXJDR-UHFFFAOYSA-N
<b>Formula:</b>	C17H11N5
<b>SMILES:</b>	<chem>N#Cc1ccc(C(c2ccc(C#N)cc2)n2cncn2)cc1</chem>
<b>Mol. weight [g/mol]:</b>	285.30
<b>CAS:</b>	112809-51-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.95		Crippen Method
logp	2.659		Crippen Method
mcvol	216.110	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C112809515&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C112809515&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/74-489-8/Letrozole.pdf>

Generated by Cheméo on 2024-05-06 21:07:10.704778928 +0000 UTC m=+17318879.625356240.

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