

# Estazolam

**Other names:**

4H-[1,2,4]Triazolo[4,3-a][1,4]benzodiazepine, 8-chloro-6-phenyl-  
D 40TA  
Eurodin  
Julodin  
4H-s-Triazolo(4,3-a)(1,4)benzodiazepine, 8-chloro-6-phenyl-  
8-Chloro-6-phenyl-4H-s-triazolo(4,3-a)(1,4)benzodiazepine  
8-Chloro-6-phenyl-4H-(1,2,4)triazolo(4,3-a)(1,4)benzodiazepine  
Esilgan  
Nuclalon  
ProSom  
Abbott-47631  
Cannoc  
Nemurel  
Somnatrol  
NSC 290818  
U 33737  
Alprazolam M (hydroxy-)-CH<sub>2</sub>O

**Inchi:**

InChI=1S/C16H11ClN4/c17-12-6-7-14-13(8-12)16(11-4-2-1-3-5-11)18-9-15-20-19-10-21

**InchiKey:**

CDCHDCWJMGXXRH-UHFFFAOYSA-N

**Formula:**

C<sub>16</sub>H<sub>11</sub>ClN<sub>4</sub>

**SMILES:**

Clc1ccc2c(c1)C(c1cccc1)=NCc1nncn1-2

**Mol. weight [g/mol]:**

294.74

**CAS:**

29975-16-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.48		Crippen Method
logp	3.272		Crippen Method
mccvol	206.320	ml/mol	McGowan Method
rinpol	2893.00		NIST Webbook
rinpol	2855.00		NIST Webbook
rinpol	2930.00		NIST Webbook
rinpol	2987.80		NIST Webbook
rinpol	2897.00		NIST Webbook
rinpol	2893.00		NIST Webbook
rinpol	2897.00		NIST Webbook

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C29975164&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C29975164&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>
<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>

# 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
<b>rinpol:</b>	Non-polar retention indices

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