

Anastrozole

Other names:	Arimidex 1,3-Benzenediacetonitrile, «alpha»1, «alpha»1, «alpha»3, «alpha»3-tetramethyl-5-(1H-1,2,4-triazol-1-ylmethyl)- 1,3-Benzenediacetonitrile, a1,a1,a3,a3-tetramethyl-5-(1H-1,2,4-triazol-1-ylmethyl)-
Inchi:	InChI=1S/C17H19N5/c1-16(2,9-18)14-5-13(8-22-12-20-11-21-22)6-15(7-14)17(3,4)10-19
InchiKey:	YBBLVLTVTVSKRW-UHFFFAOYSA-N
Formula:	C17H19N5
SMILES:	CC(C)(C#N)c1cc(Cn2cncn2)cc(C(C)(C)C#N)c1
Mol. weight [g/mol]:	293.37
CAS:	120511-73-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.92		Crippen Method
logp	2.929		Crippen Method
mcvol	239.870	ml/mol	McGowan Method

Sources

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=C120511731&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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