

Didesethylflurazepam

Other names:	2H-1,4-Benzodiazepin-2-one, 1,3-dihydro-1-(2-aminoethyl)-7-chloro-5-(2-fluorophenyl)- 1-(2-Aminoethyl)-7-chloro-5-(2-fluorophenyl)-1,3-dihydro-2H-1,4-benzodiazepin-2-one RO 7-1986 2H-1,4-Benzodiazepin-2-one, 1-(2-aminoethyl)-7-chloro-5-(2-fluorophenyl)-1,3-dihydro- 2H-1,4-Benzodiazepin-2-one, 1-(2-aminoethyl)-7-chloro-5-(o-fluorophenyl)-1,3-dihydro- Desalkylflurazepam Dideethylflurazepam Dealkylflurazepam N,N-Bisdesethylflurazepam
Inchi:	InChI=1S/C17H15ClFN3O/c18-11-5-6-15-13(9-11)17(12-3-1-2-4-14(12)19)21-10-16(23)2
InchiKey:	MVAUDJDXZPBWOW-UHFFFAOYSA-N
Formula:	C17H15ClFN3O
SMILES:	<chem>NCCN1C(=O)CN=C(c2ccccc2F)c2cc(Cl)ccc21</chem>
Mol. weight [g/mol]:	331.77
CAS:	17617-59-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.70		Crippen Method
logp	2.622		Crippen Method
mcvol	233.230	ml/mol	McGowan Method
rinpol	2660.00		NIST Webbook
rinpol	2660.00		NIST Webbook

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=C17617593&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
rinpol:	Non-polar retention indices

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