Alprazolam

Other names:

4H-[1,2,4]Triazolo[4,3-a][1,4]benzodiazepine, 8-chloro-1-methyl-6-phenyl-
4H-s-Triazolo(4,3-a)(1,4)benzodiazepine, 8-chloro-1-methyl-6-phenyl-
8-Chloro-1-methyl-6-phenyl-4H-[1,2,4]triazolo[4,3-a] [1,4]-benzodiazepine (alprazolam)
8-Chloro-1-methyl-6-phenyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine
8-Chloro-1-methyl-6-phenyl-4H-s-triazolo(4,3-a)(1,4)benzodiazepine
Alcelam
Alpaz
Alplax
Alpram
Alprazolam intensol
Alzam
Anpress
Apo-Alpraz
Constan
D 65MT
Frontal
Kalma
Panix
Prinox
Relaxol
Solanax
TUS-1
Tafil
Tafil D
Trankimazin
Tranquinal
Tricalma
U 31889
Valeans
Xanagis
Xanax
Xanax TS
Xanolam
Xanor
Zolam
Zolarem
Zoldac
Zopax
Zopic
Zotran

Inchi: InChI=1S/C17H13ClN4/c1-11-20-21-16-10-19-17(12-5-3-2-4-6-12)14-9-13(18)7-8-15(14)
InchiKey: VREFGVBLTWBCJP-UHFFFAOYSA-N
Formula: C17H13ClN4
SMILES: Cc1nnc2n1-c1ccc(Cl)cc1C(c1ccccc1)=NC2
Mol. weight [g/mol]: 308.76
CAS: 28981-97-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.43		Aqueous Solubility Prediction Method
logp	3.580		Crippen Method
mcvol	220.410	ml/mol	McGowan Method
rinpol	2936.00		NIST Webbook
rinpol	2908.00		NIST Webbook
rinpol	2910.00		NIST Webbook
rinpol	2910.00		NIST Webbook
rinpol	2936.00		NIST Webbook
rinpol	2936.00		NIST Webbook
rinpol	3243.20		NIST Webbook
tf	502.27	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	32.00	kJ/mol	501.80	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C28981977&Units=SI

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point