6-Aza-B-homo-5«alpha»-cholestano[6,7-d]tetrazol

Other names: 6-Aza-«beta»-homo-5«alpha»-cholestano[6,7-d]tetrazole
Inchi: InChI=1S/C27H46N4/c1-18(2)9-8-10-19(3)21-12-13-22-20-17-25-28-29-30-31(25)24-11-
InchiKey: NYTLYQYMYXRCEM-UHFFFAOYSA-N
Formula: C27H46N4
SMILES: CC(C)CCCC(C)C1CCC2C3Cc4nnnn4C4CCCCC4(C)C3CCC12C
Mol. weight [g/mol]: 426.68
CAS: 66233-39-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.65		Crippen Method
logp	6.872		Crippen Method
mcvol	368.310	ml/mol	McGowan Method
rinpol	3124.00		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=C66233394&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices