Triazolam M (hydroxy-)

Inchi: InChI=1S/C17H12Cl2N4O/c1-9-21-22-16-17(24)20-15(11-4-2-3-5-13(11)19)12-8-10(18)6
InchiKey: YUQRFPYHTPARRM-UHFFFAOYSA-N
Formula: C17H12Cl2N4O
SMILES: Cc1nnc2n1-c1ccc(Cl)cc1C(c1ccccc1Cl)=NC2O
Mol. weight [g/mol]: 359.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.36		Crippen Method
logp	3.724		Crippen Method
mcvol	238.520	ml/mol	McGowan Method
rinpol	3200.00		NIST Webbook
rinpol	3200.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R313565&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.